Doctoral Thesis

Techno-economic and environmental assessment of PEM water electrolysis for green H_2 production

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School of Energy and Chemical Engineering
(Chemical Engineering)

Ulsan National Institute of Science and Technology

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Approved by

Advisor

Hankwon Lim

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04.27.2021 of submission

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Abstract

With the increased interest in environmental issues, green H_2 production technology, which split H_2O into H_2 and O_2, using electricity generated from renewable energy sources, has received much attention to de-carbonize the energy production and to achieve carbon neutrality by 2050. Green H_2 is a carbon-free energy carrier, but higher unit H_2 production cost from green H_2 production owing to the high water electrolysis system price as well as the levelized cost of electricity generated from renewable energy sources than one from grey H_2 production (i.e., methane steam reforming without carbon capture and storage), is to be solved for the realization of green H_2 society. Therefore, a techno-economic assessment was conducted for green H_2 production by polymer electrolyte membrane water electrolysis using electricity generated from solar photovoltaic, onshore wind, and hydropower, to identify the effect of electrochemical parameters on H_2 yield, to assess the economic feasibility for current and future level based on process simulation results, and to identify how to make this technology cost-competitive by considering scale-up, technology development of polymer electrolyte membrane water electrolysis system, manufacturing cost reduction by learning-by-doing effect, and the decrease in levelized cost of electricity, increasing in the installed renewable energy capacity, in terms of capital and operating cost reduction in this work.

Based on techno-economic analysis results, economic parity analysis on green H_2, which is a switching point to be equal or less than unit H_2 production cost from green H_2 production compared to one from grey H_2 production, was performed to investigate when H_2 parity can occur and then it can be clearly shown that only green H_2 production using solar photovoltaic-based electricity happens to H_2 parity in approximately 2040 and 2025, in current and future level, respectively.

In addition, life cycle assessment was carried out to identify the environmental impacts such as CO_2 emission for global warming, ozone depletion, and fine particular matter formation, for overall green H_2 production through SimaPro and find out hot-spot to account for the large portion of total environmental impacts for the entire process.

From life cycle assessment results, green H_2 production using hydropower-based electricity is higher CO_2 emissions than other renewable energy sources (solar photovoltaic and onshore wind) as well as even grey H_2 production. Onshore wind is the best candidate as a renewable energy source for electricity generation, in terms of environmental impact.

Taken together, the analytic hierarchy process, which is one of the multi-criteria decision analyses, was conducted to determine the appropriate renewable energy source for green H_2 production by polymer electrolyte membrane water electrolysis based on different weighted values of techno-economic and environmental results, under determination and uncertainty.

From analytic hierarchy process results, it can be shown that onshore wind is the attractive renewable energy source for green H_2 production, when considering techno-economic and environmental aspects, simultaneously, although the best alternative should be changed according to the weighted value of criterion. Furthermore, hydropower is the most suitable renewable energy source for green H_2 production at the current level, when economic feasibility is the important factor, because the levelized cost of electricity from hydropower is cheaper than others at the current level, resulting in the lower unit H_2 production cost. However, the higher levelized cost of electricity due to the lower installed hydropower capacity as well as environmental issues can lead to the worst alternative to the renewable energy source for green H_2 production at the future level. In the same way, relatively higher CO_2 emission can result in the second alternative for solar photovoltaic, when considering high weighted values of environmental criterion, although green H_2 production using solar photovoltaic-based electricity has the lowest unit H_2 production cost in the future.

Therefore, techno-economic analysis, as well as environmental impact assessment results, should be taken into account, simultaneously, to determine the most appropriate renewable energy source for green H_2 production by polymer electrolyte membrane water electrolysis.

Acknowledgments

I would like to express my sincere appreciation to my advisor, Dr. Hankwon Lim. He has expertly guided me through my graduate education and brought out the best in me. His unwavering enthusiasm for chemical engineering kept me constantly doing my research and his generosity helped make my Ph.D. course happy.

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I really thank my parents, Giljae Lee and Younghi Lee, my brother, Jeongwan Lee, for their praise and encouragement.

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Nomenclature

AEM: Anion Exchange Membrane

ASPEN: Advanced System for Process ENgineering

BOP: Balance of Plant

CCM: Catalyst-coated membrane

CRF: Capital recovery factor

ELECNRTL: Electrolyte non-random two-liquid

HVV: Higher heating value

LCOE: Levelized cost of electricity

MSR: Methane steam reforming

O&M: Operating & maintenance

PEM: Proton exchange membrane

PSA: Pressure swing adsorption

PV: Photovoltaic

1. Introduction

1.1. Why is green H_2 important?

The anthropogenic CO_2 is emitted from electricity and heat production, transportation, industry, and so on, as shown in Fig. 1, and transport and its emission has been increased since the industrial revolution [1].

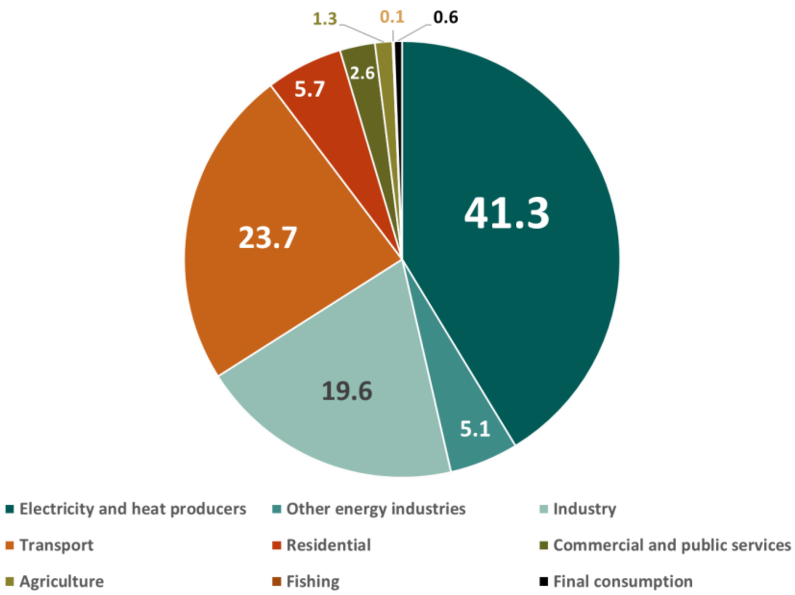


Fig. 1. Global CO_2 emission by sector [1]

According to the Our world in Data, total global CO_2 emission by fossil fuels in 2019 is approximately 36.44 billion tons accounting for 40.3% of coal, 34.1% of oil, 20.5% of gas, and 4.1% of cement, and is approximately 18.7 times compared with the one in 1900 (1.95 billion ton) [2]. In addition, the annual anomaly of the global average surface temperature in 2020 released by the National Aeronautics and Space Administration / Goddard Institute of Space Studies is 1.02 ºC. In this context, the reduction of greenhouse gases including CO_2 should be done because the global temperature to 1.5 ºC should be limited (i.e., 45% of global greenhouse gases should be reduced by 2030, compared with the one in 2010) to prevent serious environmental issues caused by global warming [3].

Global warming, which is one of the top 10 most important global environmental issues of 2020 that need to resolve, encompasses not only global climate change but also natural disaster, extreme climate events, the destruction of wildlife habitats, and the sea level rise, and many countries have put a lot of effort into the decrease in the greenhouse gases emission [4]. To decrease the emissions of greenhouse gas, Republic of Korea government set the goal of 37% of CO_2 emission reduction based on business as usual in 2030 at COP 21 in Paris and recently announced 'Renewable energy 3020 plan', which is the goal of an increase in the use of renewable energy to 20% by 2030 [5]. Furthermore, the H_2 economy is of growing importance to accelerate sustainable energy innovation according to the 2019 G20 summit held in Japan [6].

An H_2 has been already spotlighted in the world as the promising sustainable energy carrier due to the only water (H_2O) emission during combustion. Fig .2 shows the global H_2 demand from 1975 to now [6] and global H_2 demand in 2018 has approximately 4 times higher than 1975 (18.15 Mt). Furthermore, global H_2 demand will be expected to increase because the current development in H_2 fuel cells makes clean electricity generation and transportation for de-carbonization possible.

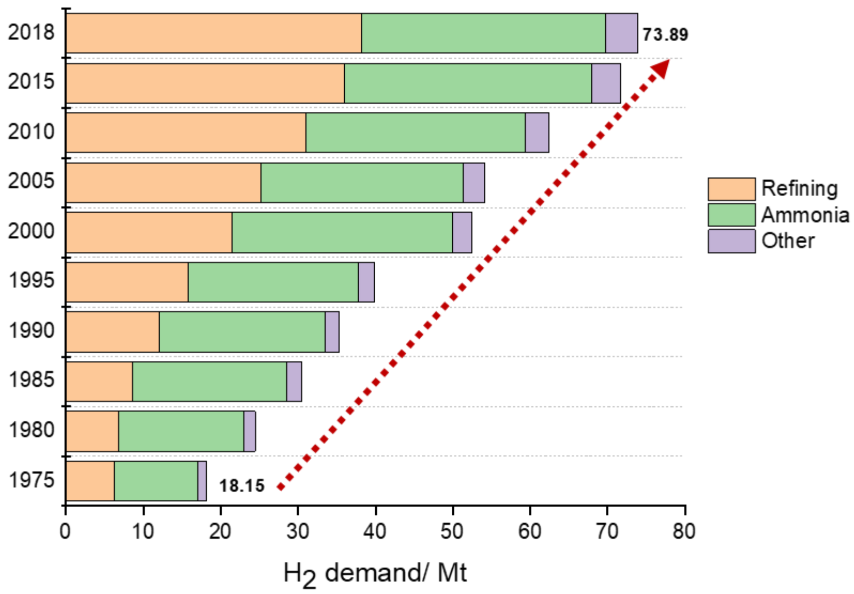


Fig. 2. Global H_2 demand [6]

However, the majority of international H_2 production methods is methane steam reforming (MSR), which is responsible for approximately 50% of one as shown in Fig. 3 [7]. Even H_2 production from water electrolysis counting less than 4% of H_2 production is mainly obtained from the by-product of chlor-alkali process by the electrolysis of brine [8].

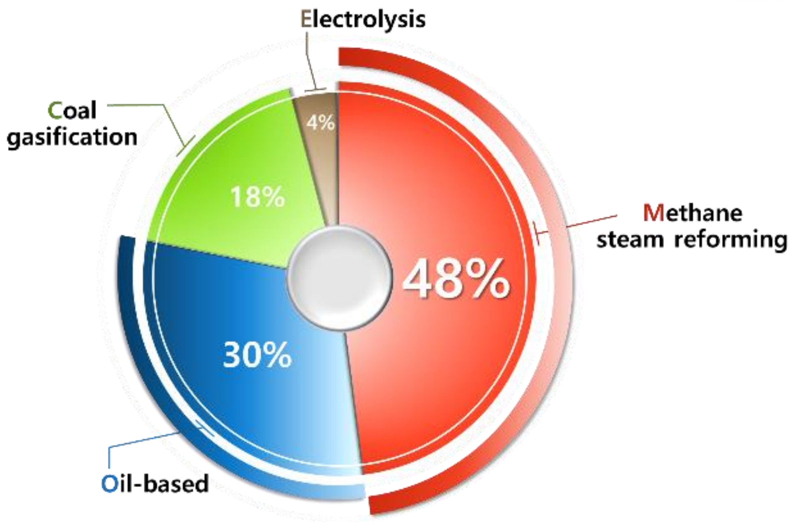


Fig. 3. International H_2 production methods [7]

Here, overall MSR is composed of both processes: MSR (Equation 1) and water gas shift reaction (Equation 2) as shown in Fig. 4.

$$CH_4 + H_2O \rightarrow CO + 3H_2 \tag{1}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{2}$$

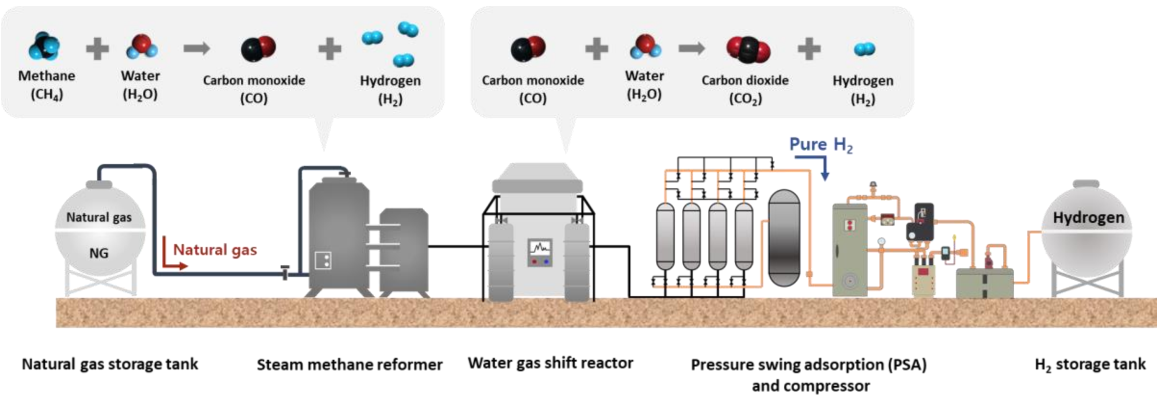


Fig. 4. Overview of methane steam reforming

In methane steam reforming, methane (CH_4), which is a major component (70-90%) of natural gas, and steam react to produce H_2 and carbon monoxide (CO), and then CO and steam are converted into additional H_2 and carbon dioxide (CO_2) in water gas shift reaction. After both processes, H_2 purification is performed to obtain the pure H_2 (99.999%) via pressure swing adsorption (PSA). Here, PSA is for adsorption of impurities (others except for H_2) from products by using adsorbent at high pressure and then impurities desorb at low pressure. Because of these reasons, the methane steam reforming system requires mainly large-scale (i.e. central H_2 production of more than 50,000 $kgH_2\ d^{-1}$). Although methane steam reforming is the most common commercial H_2 production method, there are several main drawbacks: (1) high energy requirement because methane steam reforming is the endothermic process to absorb heat, (2) CO_2 emission from the product for methane steam reforming, and direct fossil fuel gas consumption for the required energy, and (3) additional requirement of H_2 purification equipment resulting in significant cost increase. Especially, CO_2 emitted from the methane steam reforming process (about 12 kg CO_2 kg H_2^{-1}) accounts for approximately 3% of the international industrial sector [9]. Therefore, clean and sustainable H_2 production should be considered. Fig. 5 presents diverse H_2 types by distinguishing them by color, classified them into different H_2 production sources and methods. Through Fig. 5, green H_2 produced from water electrolysis using renewable energy-based electricity would be the global H_2 production pathway that we want, for carbon-free fuel production. Here, four H_2 types are classified into H_2 production methods and sources and distinguished by color as shown in Fig. 5.

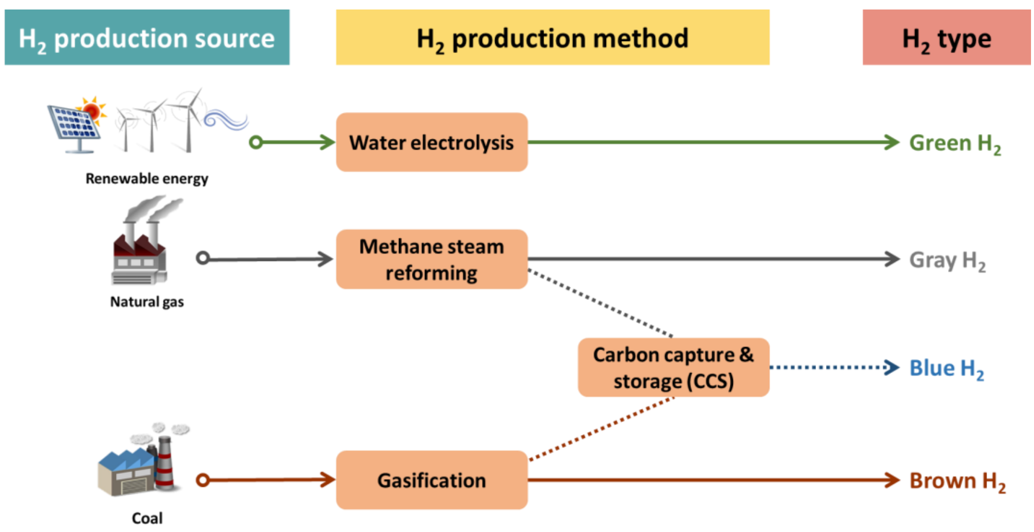


Fig. 5. H_2 production processes

However, economic issues of green H_2 production make this technology challenging to become commercialization because of high unit H_2 production cost compared to one from the conventional method. Therefore, economic analysis was covered to obtain current unit H_2 production cost for green H_2 production as well as how to make it cost-competitive compared to conventional one by scenario analysis considering diverse economic parameters such as experience rate of water electrolyzer, cost reduction of water electrolysis system resulted in technology development, and the reduction of LCOE corresponding to the increase in the installed renewable energy capacity. Furthermore, a life cycle assessment was also conducted to identify the environmental impacts such as greenhouse gas emission, ozone depletion, and particular matter formation for overall processes because the top priority of green H_2 production is sustainable in terms of technical, economic, and environmental aspects.

1.2. Water electrolysis type

Green H_2 is produced from water electrolysis using electricity generated from renewable energy sources such as solar photovoltaic, on/off-shore wind, hydropower, and geothermal. Here, water electrolysis is H_2 production by splitting H_2O into H_2 and O_2 through electricity and there are four representative water electrolysis types: alkaline water electrolysis, proton exchange membrane (PEM) water electrolysis, solid oxide electrolyzer cell and anion exchange membrane (AEM) water electrolysis as shown in Fig. 6 and Table 1 shows technical features on four water electrolysis types [10,11].

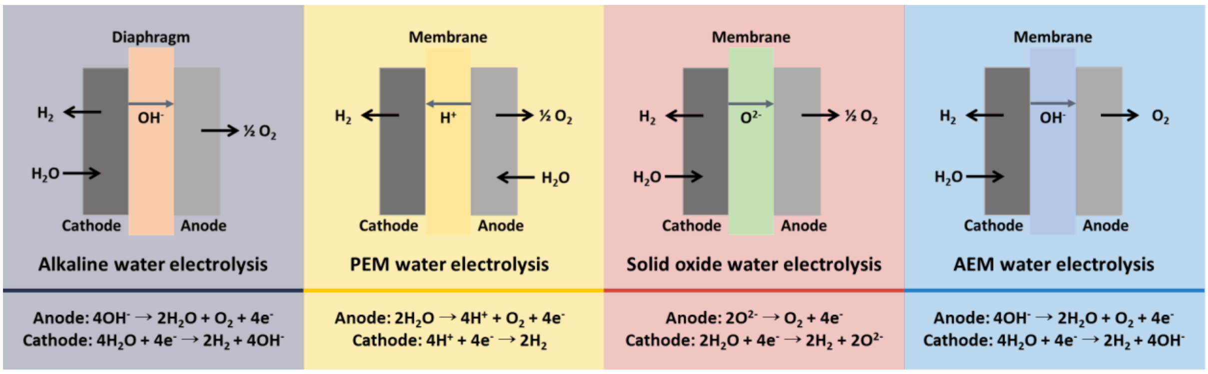


Fig. 6. Different water electrolysis types

Table 1 Technical features for four water electrolysis types [10,11]

<table>
<tr><th></th><th>Alkaline water electrolysis</th><th>PEM water electrolysis</th><th>Solid oxide electrolyzer cell</th><th>AEM water electrolysis</th></tr>
<tr><td>Electrolyte</td><td>KOH (2–30 wt%)</td><td>Solid membrane (Nafion)</td><td>Solid oxide or ceramic</td><td>Solid membrane (AS-4)</td></tr>
<tr><td>Temperature/ ℃</td><td>65–80</td><td>50–80</td><td>700–1,000</td><td>50–60</td></tr>
<tr><td>Pressure/ bar</td><td>1–30</td><td>60–76</td><td>1–15</td><td>1–30</td></tr>
<tr><td>Current density/ A cm^{-2}</td><td>0.2–0.4</td><td>0.6–2.0</td><td>0.3–1.0</td><td>0.2–1.0</td></tr>
<tr><td>H_2 production rate/ Nm^3 h^{-1}</td><td>< 1,400</td><td>< 400</td><td>< 10</td><td>< 1</td></tr>
<tr><td>Cold start-up</td><td>1–2 h</td><td>5–10 min</td><td>Hours</td><td rowspan="2">Not available</td></tr>
<tr><td>Warm start-up time</td><td>1–5 min</td><td>< 10 s</td><td>15 min</td></tr>
<tr><td>H_2 purity</td><td>> 99.5</td><td>> 99.9999</td><td>(> 99.9)</td><td>(> 99.99)</td></tr>
<tr><td>Life time/ kh</td><td>60–100</td><td>20–60</td><td>(8–20)</td><td>Not available</td></tr>
<tr><td>Investment cost/ euro kW^{-1}</td><td>800–1,500</td><td>1,400–2,100</td><td>(> 2,000)</td><td>Not available</td></tr>
<tr><td>Technical status</td><td>Mature</td><td>Commercial (Mature for small-scale)</td><td>Pre-commercial</td><td>R&D</td></tr>
</table>

Alkaline water electrolysis is the most mature technology with the use of nickel- and cobalt-based oxides for anode and cathode materials, respectively, and liquid electrolytes of 30–40 wt% KOH or NaOH. In addition, the anode and cathode are separated by a porous diaphragm consisting of ceramic oxides or polymers. Although alkaline water electrolysis is commercialization level due to the low price with no use of a noble metal catalyst and relatively easy to handle duel to the low temperature, low current density resulting in lower H_2 production rate and longer warm/cold start-up time make this technology inappropriate for green H_2 production because in particular, long start-up time is not suitable for unstable renewable energy-based electricity.

PEM water electrolysis is the secondary mature technology with the use of IrO_2 and Pt black for anode and cathode catalysts, respectively, and Nafion material for solid electrolyte and separating H_2 and O_2 produced from cathode and anode, respectively. PEM water electrolysis can operate in relatively higher current density and high pressure leading to faster kinetics of H_2 and O_2 production, with several advantages of higher H_2 purity and energy efficiency. Furthermore, a short start-up time (i.e. fast response) is available to utilize this technology for green H_2 production because fast response should be required for green H_2 production from water electrolysis using unstable renewable energy-based electricity to prevent the explosion from cross-permeation and recover efficiency.

Solid oxide electrolyte cell is the promising water electrolysis technology with the use of lanthanum strontium manganite and Ni-doped YSZ for anode and cathode catalysts, respectively, and ZrO_2-doped YSZ for solid oxide electrolyte. Solid oxide electrolyte cells can operate at high temperatures with relatively higher energy efficiency and lower energy consumption leading to the low electricity prices required for H_2 production.

AEM water electrolysis is the technology based on alkaline water electrolysis with the replacement of the conventional diaphragm with several advantages such as the use of a transition metal catalyst instead of noble metal as a catalyst, the utilization of distilled water, or a low concentration of the alkaline solution, the use of inexpensive membrane than Nafion-based membrane, and no corrosive liquid electrolyte, by strengthening the advantage of alkaline water electrolysis and supplementing the advantage of PEM water electrolysis.

In this work, PEM water electrolysis is more suitable for green H_2 production than other technologies because this technology using unstable electricity generated from renewable energy sources is covered.

1.3. Literature survey on water electrolysis technology

With the rising environmental concern on global warming, many studies regarding H_2 energy have been conducted and Fig. 7 shows the number of annual publications that are listed in "Web of Science Database" for keyword (hydrogen energy) within 10 years.

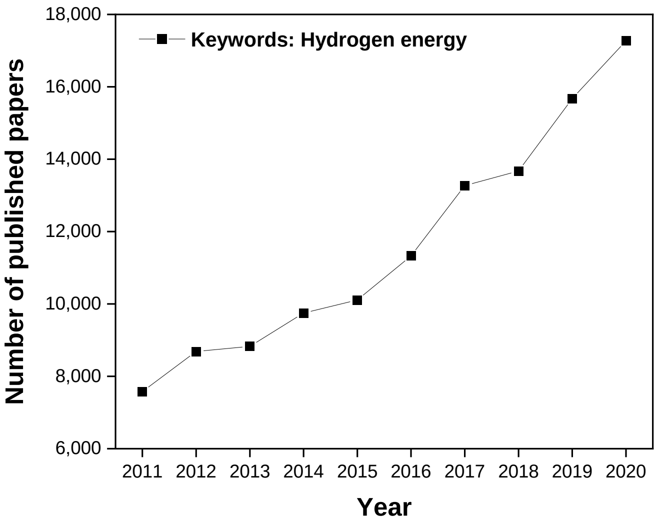


Fig. 7. The number of publications from 2011 to 2020 with the specified keyword of hydrogen energy.

From Fig. 7, the growing research trend of “H_2 energy” can be clearly confirmed with an approximately threefold higher number of published papers in 2020 than in 2011. In addition, many companies and national labs have developed water electrolysis technology, which is electrochemical-based H_2 production, to scale the H_2 production rate up and to improve technical performance (such as efficiency, current density, active area, and so on). Moreover, Fig. 8 indicates the annual number of papers published within the last five years, obtained from Web of Science according to the different keywords: keyword 1 is H_2 energy and PEM water electrolysis, keyword 2 is H_2 energy and PEM water electrolysis, economic analysis, keyword 3 is H_2 energy and PEM water electrolysis, environmental assessment, and keyword 4 is H_2 energy and PEM water electrolysis, economic analysis and environmental assessment.

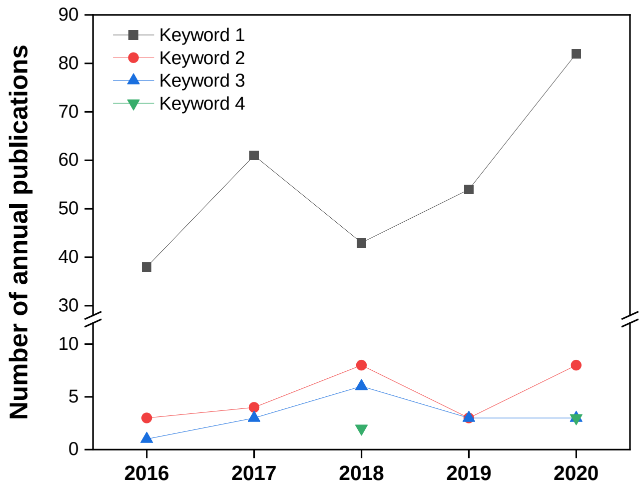


Fig. 8. Keyword analysis results on the number of annual publications with different keywords within five years.

In particular, there are two and three papers with keyword 4, in 2018 and 2020, respectively, and Table 2 tabulates literature survey results on five papers with keyword 4 [12–16].

Table 2 Literature survey covering economic and environmental assessment for green H_2 production within five years [12–16]

Authors	Comments
Ghaebi et al. [12]	• Conduct energy, exergy, economic, and environmental analysis for power and H_2 production integrating city gas station (CGS), Rankine cycle (RC), absorption power cycle (APC), and PEM water electrolyzer. • Obtain the total sum unit cost of product and CO_2 emission penalty cost of 36.9 \$ GJ^{-1} and 0.033 \$ yr^{-1} for the combined CGS/PEM water electrolyzer-RC system and 36 \$ GJ^{-1} and 0.211 \$ yr^{-1} for the combined CGS/PEM water electrolyzer-APC system.
Mohammadi and Mehrpooya [13]	• Review the combination of water electrolyzer systems with different renewable energy sources such as solar, wind, geothermal, ocean thermal, and hydroelectric energy

	• Conclude the most promising renewable energy source is hydroelectric energy for H_2 production at the current level due to the lower unit electricity cost.
Petkov and Gabrielli [14]	• Perform economic and environmental analysis to obtain minimized annual cost and CO_2 emission for power to H_2. • Suggest the significance of Feed-in Tariff (FiT) and CO_2 taxes and confirm the importance of FiT to make power to H_2 cost-competitive.
d'Amore-Domenech et al. [15]	• Carry out multi-criteria decision analysis for green H_2 production using seawater based on economic, environmental, and social factors. • Reveal that PEM water electrolysis is the best candidate in the near term.
Lee et al. [16]	• Conduct economic and environmental assessment for PEM water electrolysis considering replacement moment and different renewable energy sources. • Identify that H_2 selling price is the most important parameter to obtain high net present value and onshore wind and hydropower energy is the promising renewable energy source for cost-competitive green H_2 production.

Although several types of research were covered regarding economic and environmental assessment for green H_2 production, there is no paper to figure out the best renewable energy source for PEM water electrolysis system through multi-criteria decision analysis based on techno-economic and environmental assessment results as well as to cover H_2 parity analysis to predict when green H_2 is feasible compared to grey H_2 production based on expectation analysis results.

In addition, Figs. 9–12 show the maximum H_2 production rate from alkaline water electrolysis [17–37], PEM water electrolysis [38–54], solid oxide electrolyzer cell [55–61], and AEM water electrolysis [62–64], respectively, operating in the industrial level.

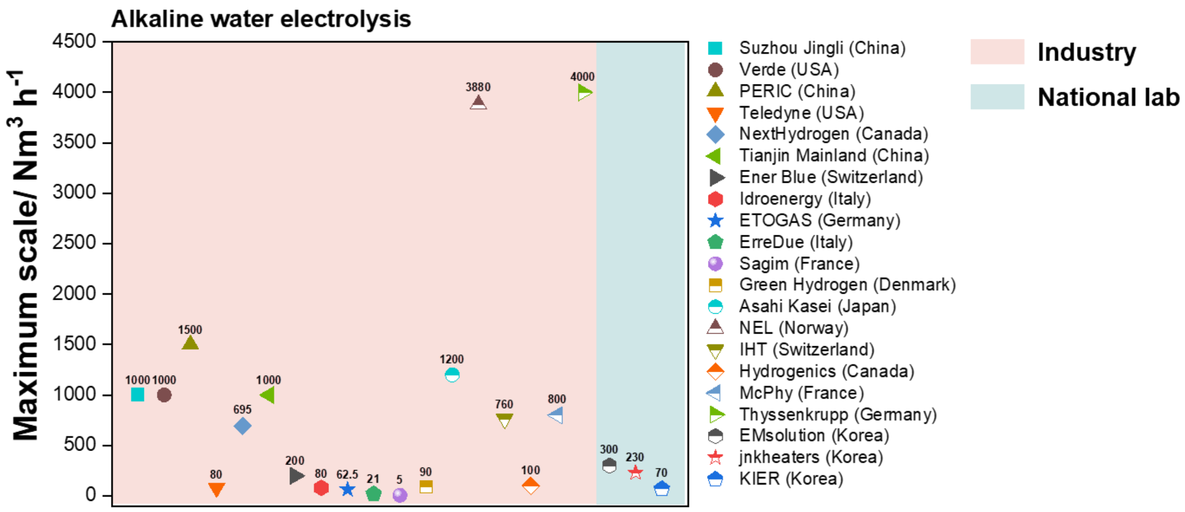


Fig. 9. Current status of development on alkaline water electrolysis in terms of maximum H_2 production scale

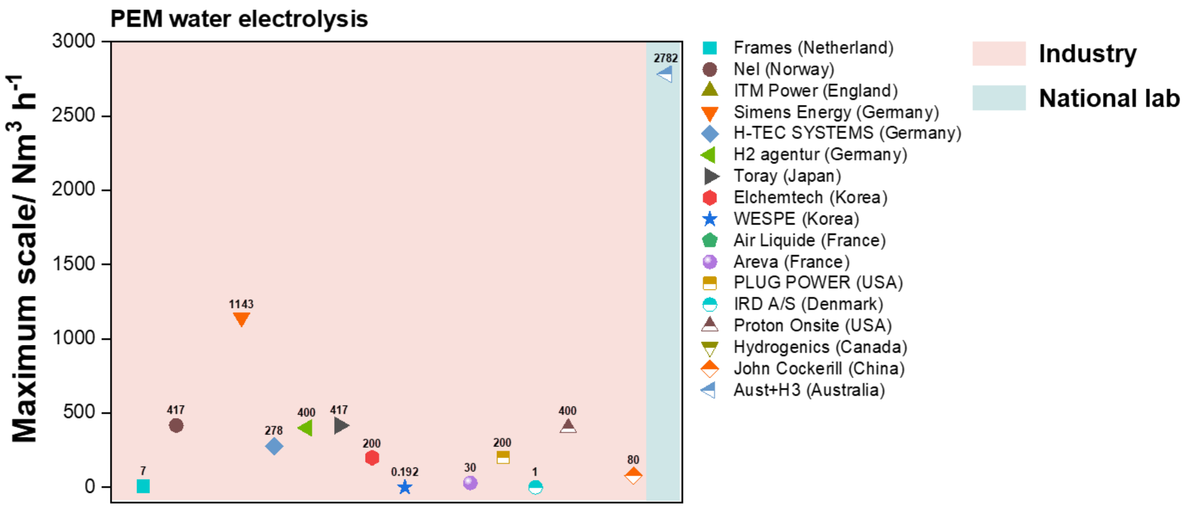


Fig. 10. Current status of development on PEM water electrolysis in terms of maximum H_2 production scale

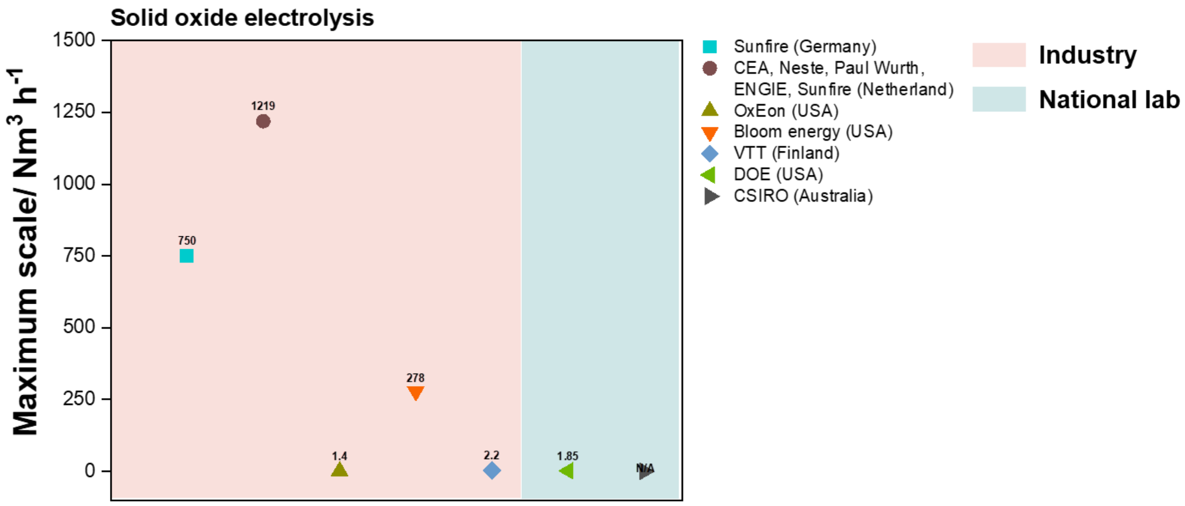


Fig. 11. Current status of development on solid oxide electrolyzer cell in terms of maximum H_2 production scale

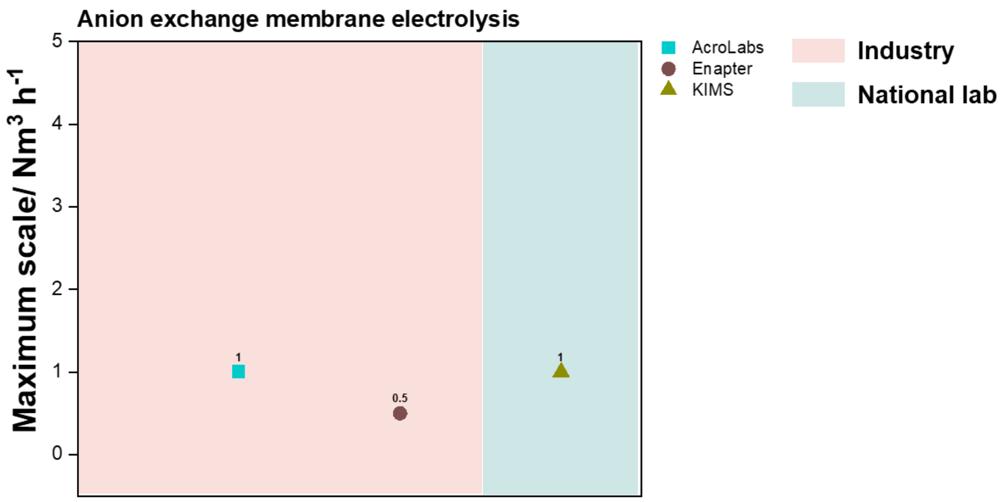


Fig. 12. Current status of development on AEM water electrolysis in terms of maximum H_2 production scale

From Figs. 9–12, the number of companies covering a certain water electrolysis type as well as maximum scale has a close relationship to the technical status of water electrolysis type. Moreover, PEM water electrolysis has already been developed on a pilot- or commercial-scale by several companies, although AWE is the most mature technology for commercial level among four water electrolysis technologies. Therefore, PEM water electrolysis was selected for green H_2 production because of the several inherent advantages of PEM water electrolysis and the possibility of scale-up.

1.4. Renewable energy source

Energy transition, which is a significant change in an energy system, is global environmental sustainability trend to realize de-carbonization of the energy sector as well as to limit the increase in global temperature by shifting fossil fuel-based energy to sustainable renewable energy, which comes from natural energy sources such as solar, wind, hydro, and others because energy production sector counts for approximately 72% of total global artificial greenhouse gas emissions [65]. In particular, Fig. 13 shows the trend of annual power capacity expansion in non-renewables and renewables, respectively, [66], showing the increased interest in renewable energy use.

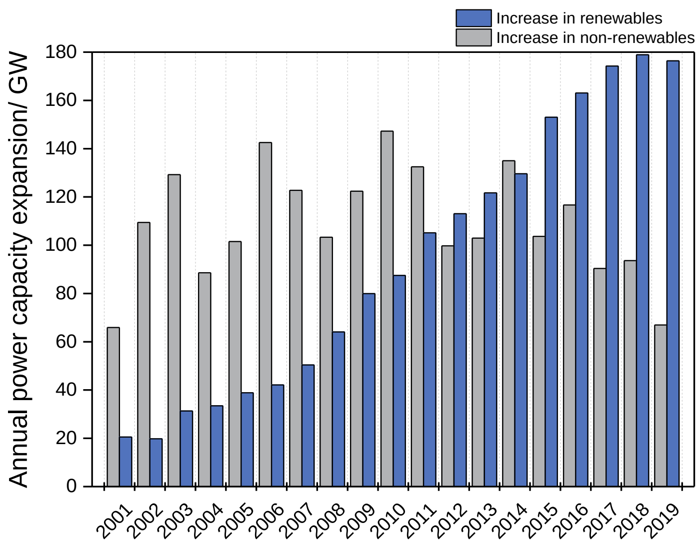
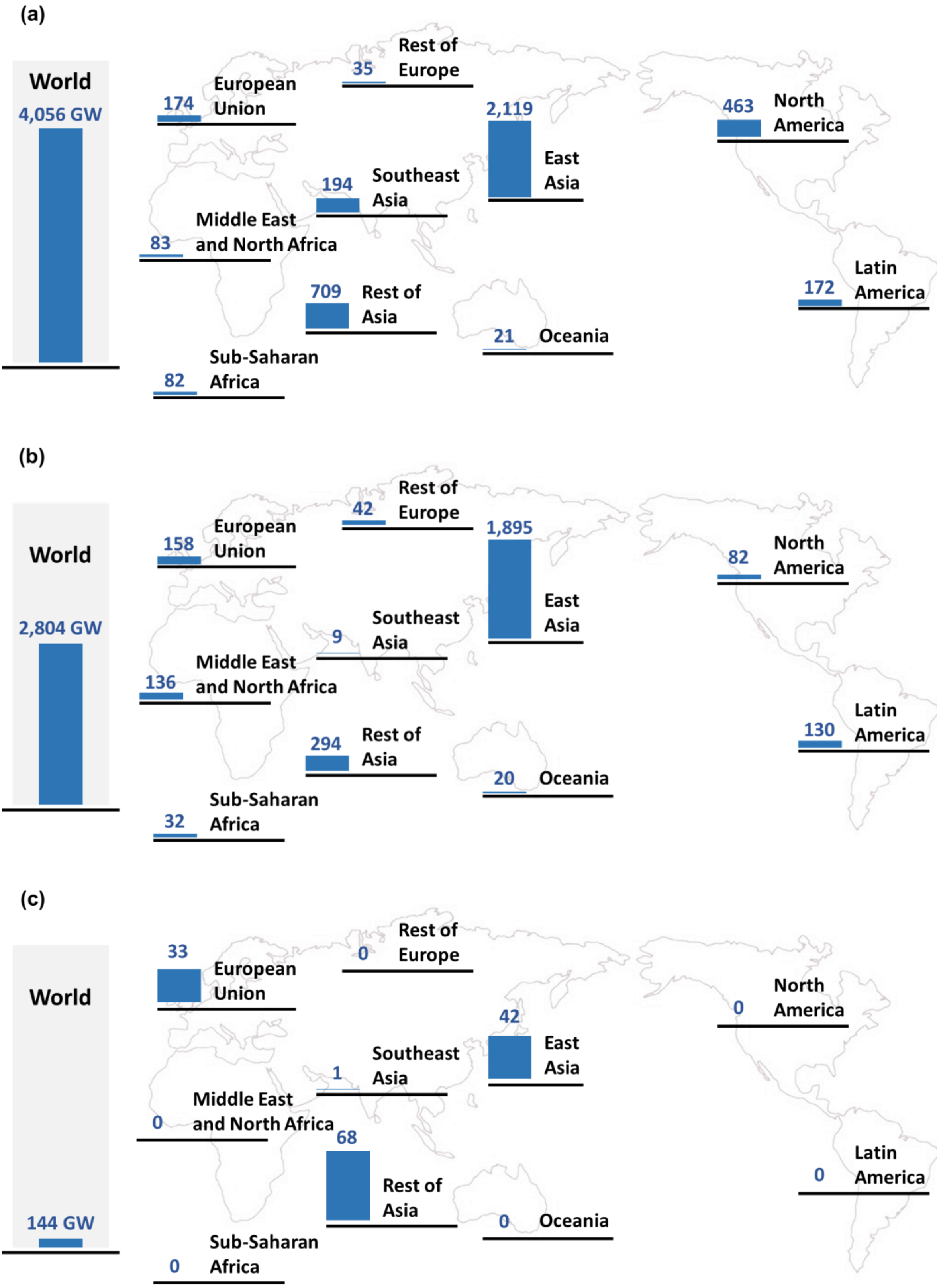


Fig. 13. Annual power capacity expansions on increases in renewables and non-renewables from 2001 to now [66].

Moreover, Fig. 14 presents the projected capacity, which the planned capacity in 2050 minus installed capacity in 2017, for electricity generation from solar photovoltaic (Fig. 14a), onshore wind (Fig. 14b), offshore wind (Fig. 14c), and hydropower (Fig. 14d).



(a)
World
4,056 GW
European Union
174
Rest of Europe
35
East Asia
2,119
North America
463
Southeast Asia
194
Middle East and North Africa
83
Latin America
172
Rest of Asia
709
Oceania
21
Sub-Saharan Africa
82
(b)
World
2,804 GW
European Union
158
Rest of Europe
42
East Asia
1,895
North America
82
Southeast Asia
9
Middle East and North Africa
136
Latin America
130
Rest of Asia
294
Oceania
20
Sub-Saharan Africa
32
(c)
World
144 GW
European Union
33
Rest of Europe
0
East Asia
42
North America
0
Southeast Asia
1
Middle East and North Africa
0
Rest of Asia
68
Latin America
0
Oceania
0
Sub-Saharan Africa
0

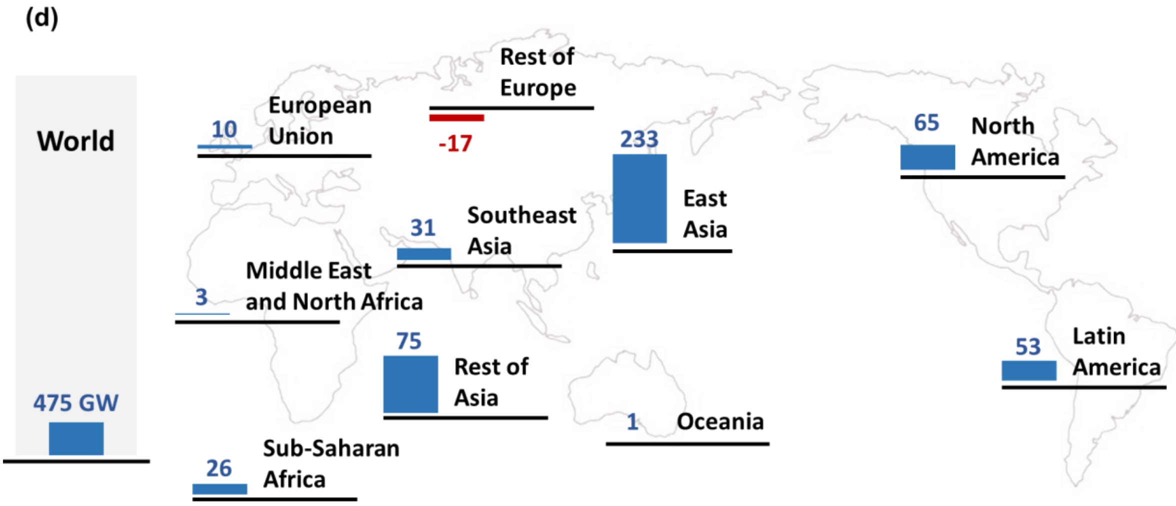


Fig. 14. The projected capacity for electricity generation from solar photovoltaic, onshore wind, offshore wind, and hydropower.

Through Fig.14, it will be expected to decrease the levelized cost of electricity (LCOE) generated from renewable energy sources corresponding to the increase in the projected capacity. Although renewable energy such as solar PV, onshore wind, hydropower, and biomass, has received much attention as low CO_2 emission technology for electricity generation, there is the challenging problem, the renewable energy demand-supply mismatch caused by the intermittent nature of inherent renewable energy properties [67]. This can lead to surplus electricity, which is undesirable consequences to require additional energy storage and therefore to result in considerable economic losses [68]. In this context, green H_2 production including renewable energy storage is in the spotlight to reach zero-CO_2 emission in the entire energy sector as well as to figure out the big problem of renewable energy.

1.5. Techno-economic and environmental assessment

Fig 15 presents the overview of techno-economic and environmental assessment including process simulation, economic analysis, and life cycle assessment.

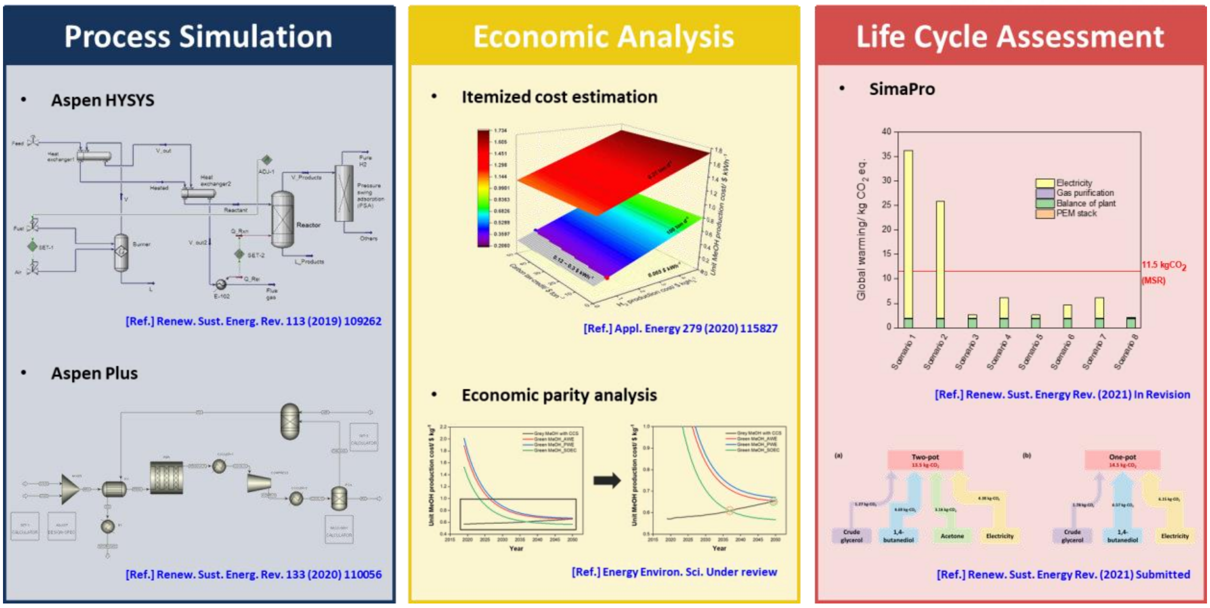


Fig. 15. The overview of techno-economic and environmental assessment

The first is process simulation. Process simulation was conducted to analyze chemical processes of interest and to find the optimized operating conditions based on mass and energy balances by using commercial process simulators, ASPEN HYSYS, or Plus (Aspen Technology, Inc., Beford, MA, USA). Here, the suitable process simulator can be selected depending on the proposed process because Aspen HYSYS is usually used for petrochemical, petrochemical refining, oil assays, and all related industry and Aspen Plus is used for fine chemistry, general chemistry, electrolytes, and so on. In particular, ASPEN (Advanced System for Process ENgineering) is based on flowsheet simulation, to model an entire chemical process including the core reactor unit, separation unit, pre-and post-treatment steps, and so on, and then design better chemical plants with profitability. Based on process simulation results, economic analysis was carried out to evaluate economic feasibility by employing several economic analysis methods as shown in Fig. 16, and then suggest how to reduce unit production cost and make this process cost-competitive compared to one from conventional production method if the proposed process is infeasible.

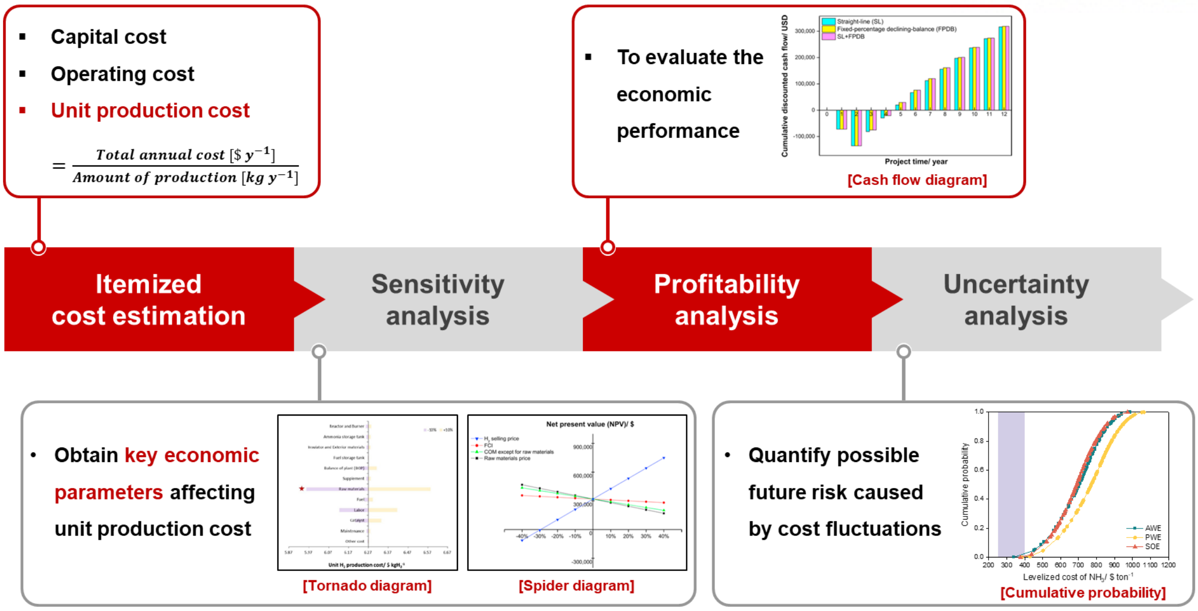


Fig. 16. The flow chart of economic analysis

Furthermore, life cycle assessment was carried out to identify the environmental impacts such as CO_2 emission, ozone depletion, particular matter formation, fossil fuel scarcity, to name a few, for overall process in terms of holistic perspective, and to find the hot-spot, which has a major impact on environmental impacts for the overall process. Taken together, multi-criteria decision analysis was done to select the best scenario or alternative for the proposed process with different weighted values of criteria under determination or uncertainty, to consider technical, economic, and environmental results, simultaneously. Therefore, techno-economic and environmental assessment for green H_2 produced from PEM water electrolysis were conducted and then multi-criteria decision analysis was performed to select the best renewable energy source based on process simulation, economic analysis, and life cycle assessment results, in terms of technical, economic, and environmental perspectives, in this work.

References

[1] Global CO_2 emissions in 2019. IEA (2020)

[2] https://ourworldindata.org/emissions-by-fuel [Accessed February 25, 2021]

[3] https://scitechdaily.com/earths-global-warming-trend-continues-2020-tied-for-warmest-year-on-record

[4] F. Liu, F. Zhao, Z. Liu, H. Hao, Can autonomous vehicle reduce greenhouse gas emissions? A country-level evaluation, *Energy Policy* 132 (2019) 462-73.

[5] D. Ko, J. Chung, K. Lee, J Park, J. Yi, Current policy and technology for Tidal Current Energy in Korea, *Energies* 12 (2019) 1807-21.

[6] The future of hydrogen. IEA for the G20, Japan 2019.

[7] B. Lee and H. Lim, Cost-competitive methane steam reforming in a membrane reactor for H_2 production: Technical and economic evaluation with a window of a H_2 selectivity, *International Journal of Energy Research* 43 (2019) 1468-1478.

[8] J. Brauns and T. Turek, Alkaline water electrolysis powered by renewable energy: A review, *Processes* 8 (2020) 248.

[9] K. Bareiß, C. de la Rua, M. Möckl, T. Hamacher, Life cycle assessment of hydrogen production from proton exchange membrane water electrolysis in future energy systems, *Applied Energy* 237 (2019) 862-872.

[10] A. Buttler and H. Spliethoff, Current status of water electrolysis for energy storage, grid balancing and sector coupling via power-to-gas and power-to-liquids: A review, *Renewable and Sustainable Energy Reviews* 82 (2018) 2440-2454.

[11] H. Miller, K, Bouzek, J. Hnat, S. Loos, C. Bernäcker, T. Weißgärber, L. Röntzsch, J. Meier-Haack, Green hydrogen from anion exchange membrane water electrolysis: a review of recent developments in critical materials and operating conditions, *Sustainable Energy Fuels* 4 (2020) 2114-2133.

[12] H. Ghaebi, B. Farhang, H. Rostamzadeh, T. Parikhani, Energy, exergy, economic and environmental (4E) analysis of using city gate station (CGS) heater waste for power and hydrogen production: A comparative study, *International Journal of Hydrogen Energy* 43 (2018) 1855-1874.

[13] A. Mohammadi, M. Mehrpooya, A comprehensive review on coupling different types of

electrolyzer to renewable energy sources, *Energy* 158 (2018) 632-655.

[14] I. Petkov,P. Gabrielli, Power-to-hydrogen as seasonal energy storage: an uncertainty analysis for optimal design of low-carbon multi-energy systems, *Applied Energy* 274 (2020) 115197.

[15] R. d'Amore-Domenech, Ó. Santiago, T.J. Leoa, Multicriteria analysis of seawater electrolysis technologies for green hydrogen production at sea, *Renewable and Sustainable Energy Reviews* 133 (2020) 110166.

[16] H. Lee, B. Lee, M. Byun, H. Lim, Economic and environmental analysis for PEM water electrolysis based on replacement moment and renewable electricity resources, *Energy Conversion and Management* 224 (2020) 113477

[17] https://www.jinglihydrogen.com/water-electrolyzer/water-electrolyzer-dq1000.html

[18] http://www.verdellc.com/JProduct.asp

[19] http://www.peric718.com/Alkaline-Type-Hydrogen-G/r-85.html

[20] http://www.teledynees.com/our-products/hydrogen-oxygen-generation-systems/titan-el

[21] https://nexthydrogen.com/products/

[22] http://www.cnthe.com/en/product_detail-35-43-30.html

[23] http://www.ener-blue.com/hydrogen-generators/outdoor

[24] https://idroenergy.it/generatori-di-idrogeno/mod-120-0/?lang=en

[25] https://reader.elsevier.com/reader/sd/pii/S136403211731242X?token=1E90D37D743F2DBFEEC0EBA839CFFC620A3F9F93F0E08CE3925DCF4D2B64F055A5BE37DD58A17E560851AB4054F11E4F

[26] https://reader.elsevier.com/reader/sd/pii/S136403211731242X?token=1E90D37D743F2DBFEEC0EBA839CFFC620A3F9F93F0E08CE3925DCF4D2B64F055A5BE37DD58A17E560851AB4054F11E4F

[27] https://sagim-gip.com/en/products/

[28] https://greenhydrogen.dk/wp-content/uploads/2020/11/GHS-HyProvide-A-series-folder_web_spread.pdf

[29] http://www.h2news.kr/news/article.html?no=8206 / https://www.internationales-verkehrswesen.de/worlds-largest-single-stack-alkaline-water-electrolysis-system/

[30] https://nelhydrogen.com/product/atmospheric-alkaline-electrolyser-a-series/

[31] http://www.iht.ch/technologie/electrolysis/industry/high-pressure-electrolysers.html

[32] https://etipwind.eu/wp-content/uploads/A2-Hydrogenics_v2.pdf

[33] https://mcphy.com/en/equipment-services/electrolyzers/large/

[34] https://ucpcdn.thyssenkrupp.com/_binary/UCPthyssenkruppBAISUhdeChlorineEngineers/en/products/water-electrolysis-hydrogen-production/alkaline-water-electrolysis/link-thyssenkrupp_Hydrogen_Water_Electrolysis_and_green_chemicals.pdf

[35] http://www.yesems.co.kr/kor/business/energy_h2_generator.html#header

[36] https://www.h2news.kr/news/article.html?no=7762

[37] https://biz.chosun.com/site/data/html_dir/2020/10/13/2020101302335.html

[38] http://www.h2news.kr/news/article_print.html?no=8535

[39] https://www.prnewswire.com/news-releases/nel-asa-received-purchase-order-for-a-1-5-mw-pem-electrolyser-in-the-us-301175604.html

[40] https://www.itm-power.com/products

[41] https://new.engineering.com/story/siemens-to-build-huge-green-hydrogen-production-facility-in-germany

[42] https://www.h-tec.com/en/products/electrolyser-me-4501400/

[43] https://h2agentur.de/en/pem-electrolysis-systems/

[44] https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwiCqYf82LPtAhVPfd4KHSCWCn8QFjADegQIAxAC&url=https%3A%2F%2Ffch.europa.eu%2Fsites%2Fdefault%2Ffiles%2F210-MI_Antwerp-H2_Valleys-Japan%2520%25282%2529.pdf&usg=AOvVaw0yuTF-6B7LbhC15dNEFrMq

[45] http://www.h2news.kr/news/article.html?no=8489

[46] http://wespe.kr/ko/products/standard

[47] https://www.businesswire.com/news/home/20190224005158/en/Air-Liquide-Invests-in-the-World%E2%80%99s-Largest-Membrane-Based-Electrolyzer-to-Develop-Its-Carbon-Free-Hydrogen-Production

[48] https://www.arevah2gen.com/en/products-services

[49] https://www.ginerelx.com/electrolyzer-systems

[50] https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwi0huLq2rPtAhWcwYsBHdacCeoQFjAAegQIBBAC&url=http%3A%2F%2Fwww.kdfuelcell.net%2F-%2Fmedia%2FCentre%2FENRGK_ELE%2FKDFuelCell%2F2013-Presentations%2FIRD-KDFuelCell.ashx%3Fla%3Dda%26hash%3D8093FF192E19E745D5932E9538436D8C3821B052&usg=AOvVaw1ODDysGCQzhrQovBCzb1jP

[51] https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwiY4tf43rPtAhXty4sBHYxyAjQQFjAAegQIAxAC&url=https%3A%2F%2Fwww.protononsite.com%2Fsites%2Fdefault%2Ffiles%2F2016-10%2Fpd-0600-0115_rev_a%2520%25281%2529.pdf&usg=AOvVaw2sDO5wnsUeSVP1Ycr-seih

[52] https://etipwind.eu/wp-content/uploads/A2-Hydrogenics_v2.pdf

[53] https://www.jinglihydrogen.com/water-electrolyzer/pem-water-electrolysis.html

[54] https://physicstoday.scitation.org/doi/10.1063/PT.3.4543

[55] https://www.sunfire.de/en/green-hydrogen

[56] http://www.h2news.kr/news/article.html?no=8238

[57] https://oxeonenergy.com/projects/inl

[58] https://www.h2news.kr/news/article.html?no=8360

[59] https://static1.squarespace.com/static/584e8e06579fb3cb3269b3f6/t/5db2f924c4ca110437028b06/1572010299376/52_thomann_ICE2019.pdf

[60] https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwismNOB7b

PtAhWKA4gKHVeYDpcQFjAAegQIBBAC&url=https%3A%2F%2Fwww.hydrogen.energy.gov%2Fpdfs%2Fprogress17%2Fvii_c_4_ghezel-ayagh_2017.pdf&usg=AOvVaw3cK6v7ClJH20ekV52OBHyu

[61] http://www.uigi.com/h2_conv.html

[62] https://h2news.kr/mobile/article.html?no=7330

[63] http://www.h2news.kr/news/article.html?no=8483

[64] http://www.h2news.kr/news/article.html?no=8483

[65] Center for Climate and Energy Solutions. Global Carbon Dioxide Emissions, 1850-2040.

https://www.c2es.org/content/international-emissions/ [accessed 22 February 2021]

[66] Renewable Capacity Statistics 2020, International Renewable Energy Agency; 2020 March.

[67] G. Mul, “Iso lated low-valent nickel.”, Nature energy 3 (2018) 90-91.

[68] W. Zappa, M. Broek, “Analysing the potential of integrating wind and solar power in Europe using spatial optimization under various scenarios”, Renewable and Sustainable Energy Reviews 94 (2018) 1192-1216.

2. Techno-economic assessment

2.1. Process description

In this work, Aspen Plus V11, which is a well-known commercial process simulator (Aspen Technology, Inc., Beford, MA, USA), was used to model flowsheet of green H_2 production from PEM water electrolysis for the green H_2 production capacity of 1,500 kg d^{-1}, based on mass and energy balances. In electrochemical water splitting, the hydrogen evolution reaction ($2H^+ + 2e^- \rightarrow H_2$) is the cathodic reaction and the oxygen evolution reaction is the anodic reaction. Firstly, the electrolyte non-random two-liquid (ELECNRTL) equation of state was used because it calculates liquid phase properties from the Electrolyte-NRTL activity coefficient model. The reactant stream including water is pressurized to 30 bar and heated to 333 K, before inputting reactant in the PEM water electrolysis system. And then, the PEM water electrolysis system is modeled by using RSTOIC and calculator to consider electrochemical parameters such as faradaic efficiency, cell voltage, current density, active cell area, power density, the required energy, and the number of cells of stacks for PEM water electrolysis system [1]. Here, H_2 production flow was calculated based on faradaic efficiency, current density, cell active area, and cell numbers for the PEM water electrolysis system as shown in Equation 3.

$$H_2 = \frac{FE \times CD \times AA \times Cells \times System \times 7{,}200}{2e^- \times 96485 \times 1000} \quad (3)$$

, where H_2 is H_2 mass flow rate produced from water electrolysis ($\frac{kg}{h}$), FE is faradaic efficiency, which is the ratio of the measured amount of H_2 (or O_2) produced, and the theoretical one according to Faraday's Law, a CD is a current density ($\frac{A}{cm^2}$), AA is cell active area (cm^2), Cells is the number of cells for H_2 production (Here, 510 cells for one PEM water electrolysis system was used.), and System is the number of systems for H_2 production (Here, one PEM water electrolysis system is for 1 MW).

In addition, both current density-potential curves depending on the energy efficiency of ~70% and more than 86% (Fig. 17) were considered [1] and the required energy for the PEM water electrolysis system calculated from Equation 4 was applied to the process model.

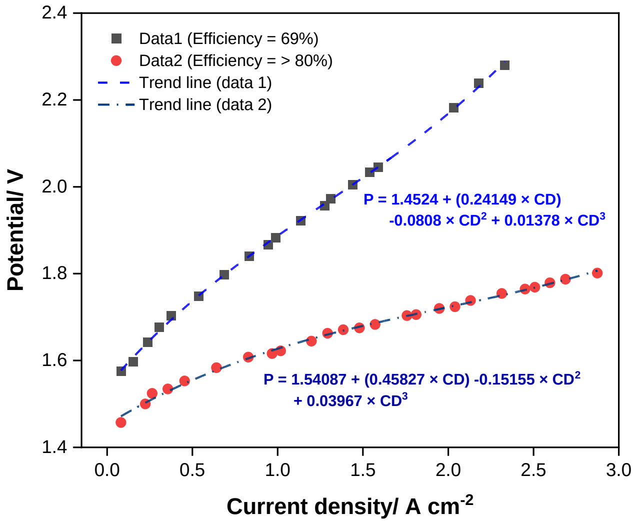


Fig. 17. Current density–Potential curve according to the energy efficiency

$$RE = \frac{CD \times P \times AA \times Cells \times System}{H_2 \times 1000} \tag{4}$$

, where RE is the required energy for PEM water electrolysis system ($\frac{kWh}{kg}$), P is potential, and H_2 is the calculated H_2 mass flow rate produced from water electrolysis ($\frac{kg}{h}$).

After the PEM water electrolysis system, H_2 produced from cathode fed into the separator to obtain high purity H_2. From the process model, the effect of current density and cell-active area (i.e., technology development) on H_2 production rate as well as the required energy was confirmed.

2.2 Economic analysis

Even though green H_2 production technology has been in the spotlight recently, with the growing interest in the environmental issues, because H_2 energy is non-toxic, clean, and sustainable, leading to lower greenhouse gas emissions than one using fossil fuels when generating the same amount of energy. However, the expensive H_2 production cost makes commercial deployment and widespread use challenging. Therefore, Economic analysis is important to commercialize new technology like green H_2 production. In this work, based on process simulation results, economic analysis was performed to obtain current unit H_2 production cost, predict future unit H_2 production cost considering the changes of LCOE, learning-by-doing effects (i.e., water electrolyzer cost reduction) corresponding to the global H_2 demand, as well as the technology development, and evaluate the economic feasibility for green H_2 production by PEM water electrolysis by using itemized cost estimation, sensitivity analysis, profitability analysis using a cash flow diagram, and uncertainty analysis employing Monte-Carlo simulation method. Moreover, H_2 parity, which is switch point due to the equal unit H_2 production costs (i.e., unit H_2 production cost from fossil fuel-based H_2 production is the same one from water electrolysis using renewable energy-based electricity) was estimated to identify the possibility for the replacement of grey or brown H_2 to green H_2, in terms of economic aspect.

2.2.1. Capital cost

Itemized cost estimation was conducted to calculate unit H_2 production cost by classifying each item into capital cost and operating cost, properly. In this work, capital cost consists of PEM water electrolysis system; PEM water electrolysis stack including catalyst-coated membrane (CCM), porous transport layer, frame, bipolar plates, assembly & end-plates, and balance of stack, and balance of plant (BOP) composed of power supplies, deionized water circulation, hydrogen processing, cooling, and miscellaneous. In this work, PEM water electrolysis systems with 10 MW capacity, were considered for green H_2 production at the current level. Operating cost is electricity price, corresponding to the amount of electricity required for the PEM water electrolysis system, and operating & maintenance (O&M) cost.

Capital cost is closely related to capacity and Equation 5 is the most common relationship between capital cost and capacity, based on previously reported data [2].

$$\mathrm{C}_2 = C_1 \times \left(\frac{\mathrm{A}_2}{\mathrm{A}_1}\right)^{\mathrm{n}} \tag{5}$$

, where Reference cost is capital cost data obtained from previously reported references. A is an annual H_2 production rate, and n is the cost exponent. In general, the six-tenths rule, which is used for cost exponent of 0.6, is often used to estimate the increase in capital cost when the capacity increases. In addition, Equation 6 is rearranged to consider the economy of scale [2].

$$\frac{C}{A} = \mathrm{K} \times A^{n-1} \tag{6}$$

When Equation 6 is plotted on log-log coordinates, a slope obtained from the resulting curve means cost exponent for equipment. Fig. 18 presents the calculating slope to obtain cost exponents for PEM water electrolysis systems with 1 MW capacity, through the trend line.

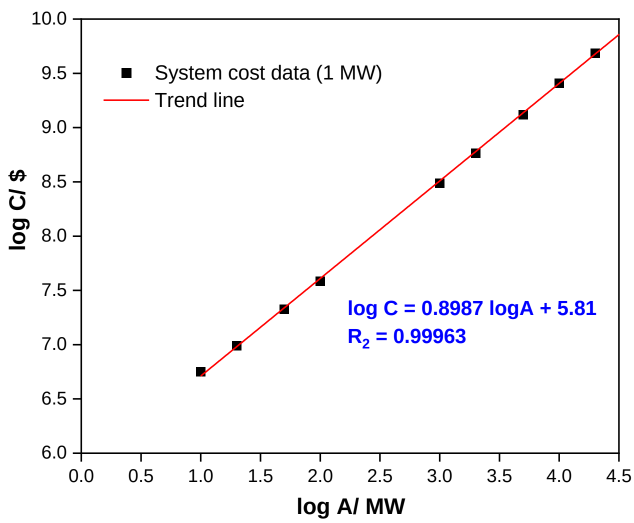


Fig. 18. Cost exponent calculation for PEM water electrolysis system with 1 MW capacity

From Fig. 18, the cost exponent of 0.8987 for PEM water electrolysis system with 1 MW capacity was obtained showing that PEM water electrolysis system experiences economies of scale related to capital cost due to the cost exponent of less than 1, resulting in lower PEM water electrolysis system price when H_2 production capacity increases. Here, the initial capital cost is the PEM water electrolysis system including the PEM water electrolysis stack and BOP with a unit of currency such as \$. To calculate unit H_2 production cost with a unit of \$ kgH_2^{-1}, it is needed to convert initial capital cost into annual one by using capital recovery factor, which is a discount factor presenting that present value is equivalent to an annual value called as capital recovery factor (CRF), based on both the interest rate and the time duration (Equation 7).

$$\mathrm{CRF} = \frac{\mathrm{i}(1+\mathrm{i})^{\mathrm{n}}}{(1+\mathrm{i})^{\mathrm{n}} - 1} \tag{7}$$

, where i is a discount rate (In this work, 4.5% of the interest rate is applied to the PEM water electrolysis system) and n is the time duration. Here, the durability of 7 years and 10 years are considered for PEM water electrolysis systems in the current and future, respectively. [3]

In this work, three methods such as 1) scale-up, 2) technology development, and 3) experience rate were considered to reduce capital cost. Here, scale-up can result in economy of scale, technology development on the efficiency of PEM water electrolysis stack can bring about higher H_2 production rate when the same electric power was consumed, and experience rate can lead to manufacturing cost reduction with the accumulated production experience (i.e., learning-by-doing effect) [4].

Experience rate was established by Wright in the early 1900s and applied to one of the capital cost reduction methods in this work. The change in PEM water electrolysis system cost with the passage of time was estimated with an inherent experience rate according to the increase in global H_2 demand in the future (Equation 8–10).

$$\frac{C_2}{C_1} = \left(\frac{P_2}{P_1}\right)^{-\alpha} = (2)^{-\alpha} \tag{8}$$

$$lr = \frac{C_1 - C_2}{C_1} = 1 - \frac{C_2}{C_1} = 1 - 2^{-\alpha} \tag{9}$$

$$\ln C_2 = -\alpha \ln\left(\frac{P_2}{P_1}\right) + \ln C_1 \tag{10}$$

, where C_2 is the estimated PEM water electrolysis system cost at the certain time, determined by the change in global H_2 demand, C_1 is the current PEM water electrolysis system cost, P_2 is the expected global H_2 demand in future, and P_1 is the current global H_2 demand, α is an experience index, and lr is an experience rate.

Although water electrolysis accounts for only 4% of the global H_2 production method as shown in Fig. 3, the percentage will be expected to increase because green H_2 is one of the pathways for carbon neutrality by 2050, which offsets the same amount of emitted CO_2 in the national economy or business by some other methods. Therefore, the percentage of H_2 production from water electrolysis was assumed of 30%, 50%, 70%, and 100%, with a proportional increase based on 4% in the current level (2018), in this work, as shown in Fig. 19.

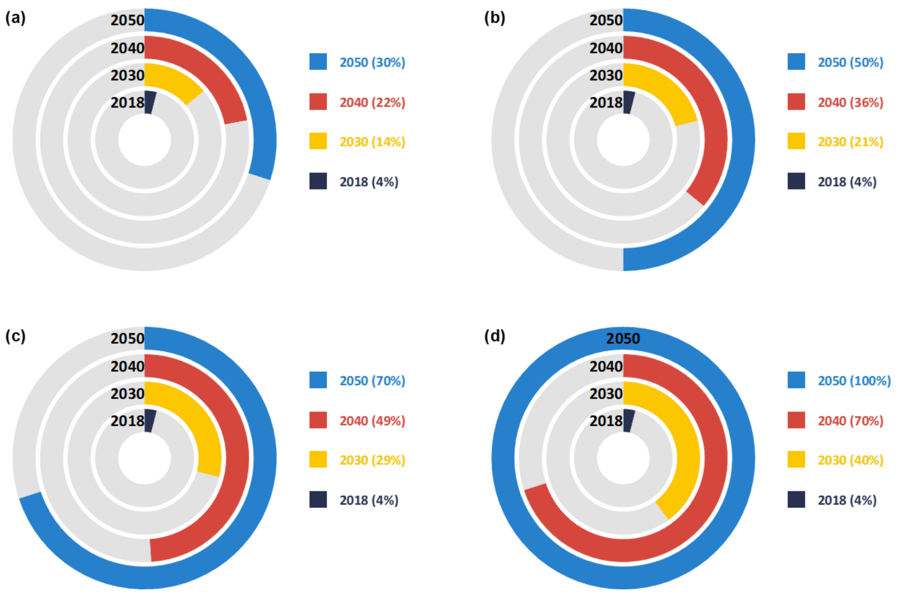


Fig. 19. Four scenarios on the percentage of H_2 production from water electrolysis.

Moreover, the global H_2 demand by 2050 through data fitting was estimated with a trend line based on historical data and predict data, as shown in Fig. 20 [5].

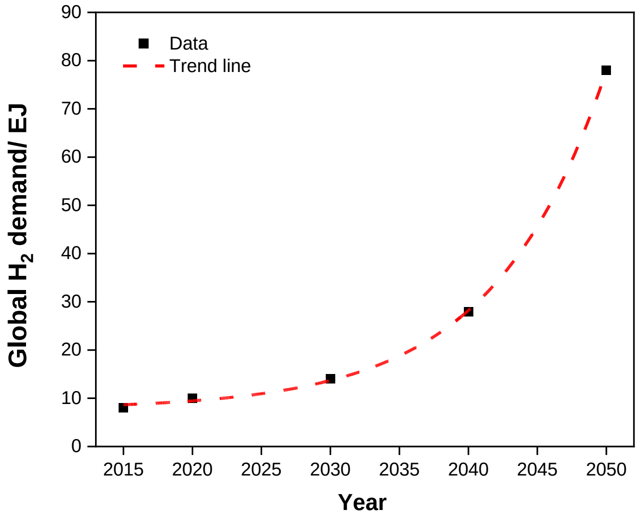


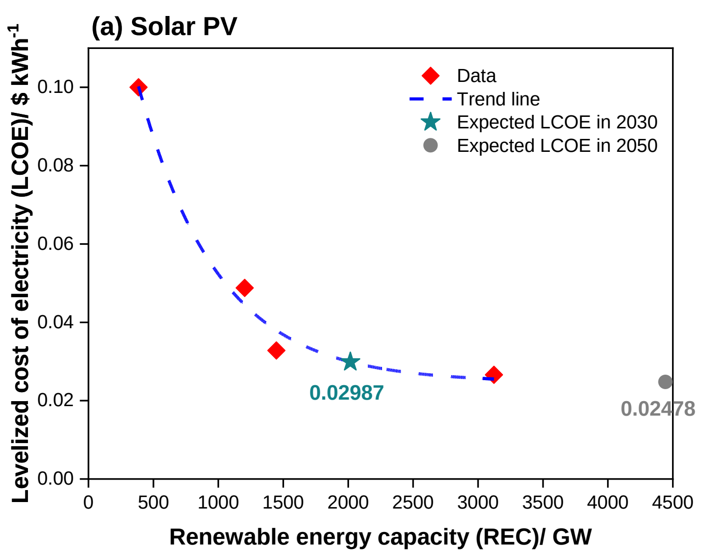
Fig. 20. Estimated global H_2 demand by 2050.

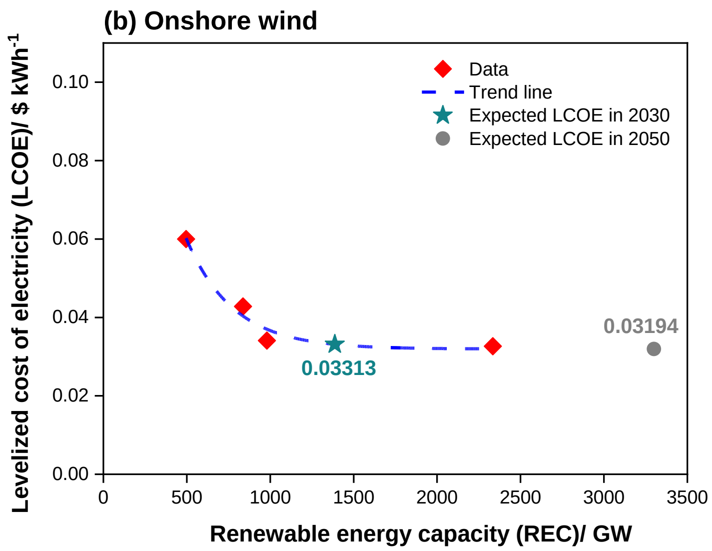
Through Fig. 20, the equation of trend line on the estimated global H_2 demand by 2050 was investigated (Equation 11).

$$\text{Global } H_2 \text{ demand} = 7.721 + 1.685 \exp((\text{Year} - 2019.73)/8.115) \quad (11)$$

2.2.2. Operating cost

Water electrolysis is reported that electricity price has the greatest impact (70–80%) on unit H_2 production cost [6]. Therefore, how to reduce the LCOE generated from renewable energy sources is crucial to reach the ultimate goal of this work. Here, solar photovoltaic (PV), onshore wind, and hydropower were considered as renewable energy sources because three renewable energy sources belong to the top five commercial renewable energy sources raked by market share and growth. In particular, LCOEs by 2050 through data fitting were estimated based on the relationship of LCOE for solar PV, onshore wind, and hydropower on the installed capacity, as shown in Fig. 21 [7].





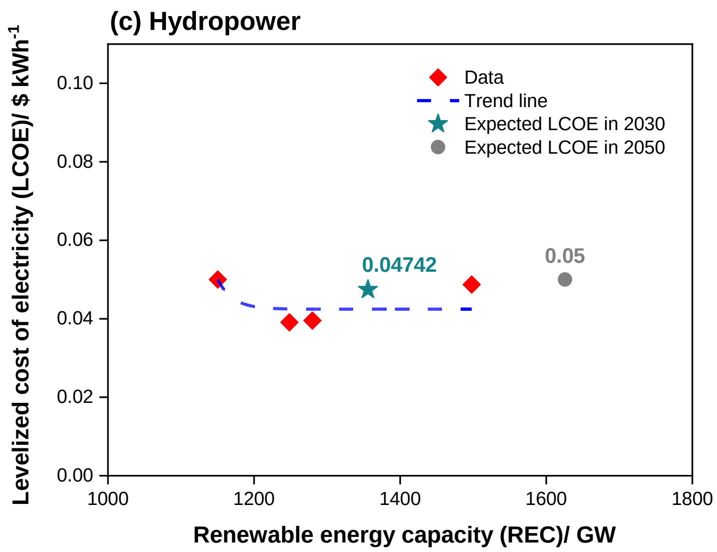


Fig. 21. Estimated levelized cost of electricity for (a) solar PV, (b) onshore wind, and (c) hydropower according to the projected renewable energy capacity.

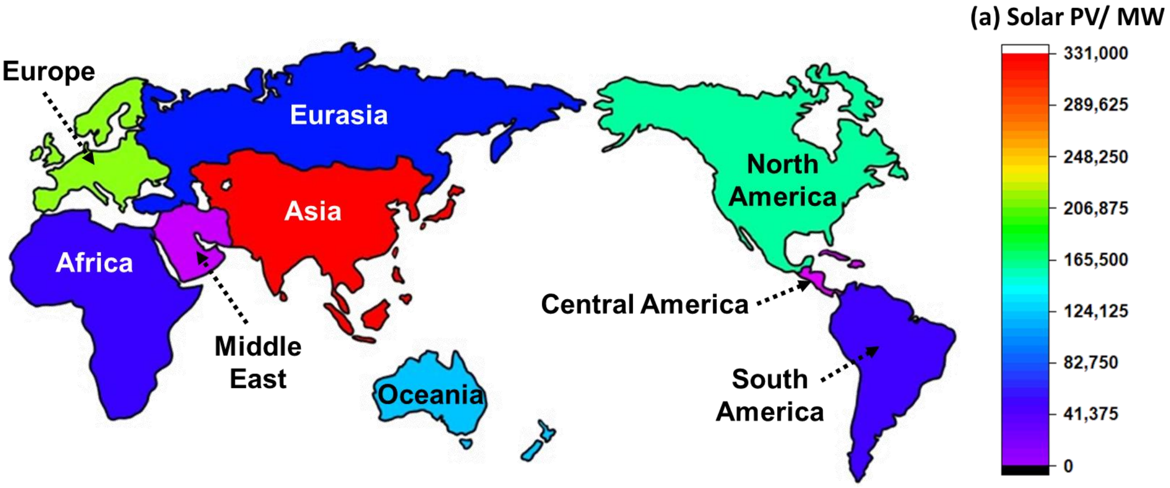
First of all, the equation of trend line on the estimated LCOEs for solar PV, onshore wind, and hydropower, was obtained (Equations 12–14).

$$\text{LCOE (Solar PV)} = 0.02468 + 0.14226 \times 0.99836^{\text{Renewable energy capacity}} \quad (12)$$

$$\text{LCOE (Onshore wind)} = 0.03194 + 0.16479 \times 0.99645^{\text{Renewable energy capacity}} \quad (13)$$

$$\text{LCOE (Hydropower)} = 0.05 - 0.0109 \times \exp(-\exp(-z)-z+1)$$
$$z = (\text{Renewable energy capacity} - 1248.30861)/83.81396 \quad (14)$$

Moreover, from Fig. 21, the estimated LCOEs in 2050 were 0.02478, 0.03194, and 0.05 \$ kWh^{-1} for solar PV, onshore wind, and hydropower, respectively, because of the higher projected capacity of solar PV in 2050 (4,056 GW) than onshore wind (2,804 GW) and hydropower (475 GW), as shown in Fig. 14. It is because the environmental and social issues such as biodiversity and land use for hydropower are to be controversial, although hydropower-based LCOE has the lowest due to the higher global hydropower-based energy generation capacity in 2018, now, (as shown in Fig. 22 [8]).



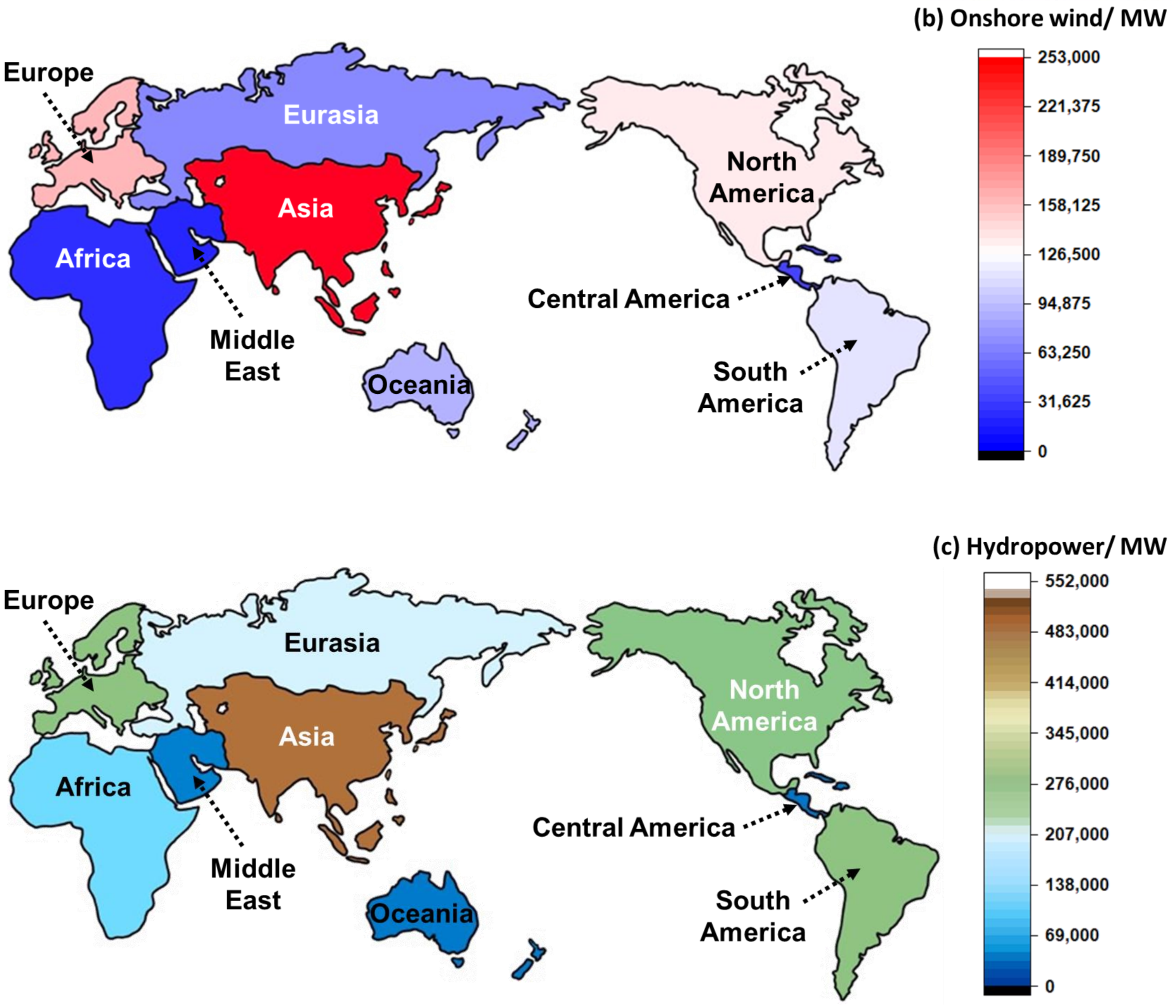


Fig. 22. Global renewable energy capacity in 2019 with the different renewable energy sources such as (a) solar photovoltaic (solar PV), (b) onshore wind, and (c) hydropower.

Finally, O&M cost assumed 4% of the initial PEM water electrolysis system cost to cover the required economic parameters when operating PEM water electrolysis system [9].

2.2.3. Unit H_2 production cost

Based on capital and operating costs for green H_2 production by PEM water electrolysis system using electricity generated from solar PV, onshore wind, and hydropower, unit H_2 production cost was calculated in Equation 15.

$$\text{Unit } H_2 \text{ production cost } = \frac{\sum_{i=1}^{n}(IC_i \times CRF_j) + \{OM \times \sum_{i=1}^{n} IC_i\} + Elec}{H_2\ yield\left(\frac{kg}{h}\right) \times 24 \times 365 \times SF}, \tag{15}$$

, where IC_i is the initial CAPEX, including PEM water electrolysis stack and BOP, CRF_j is the calculated CRF values according to the lifetime of j (used 0.1921 for current and 0.1492 for future), OM is the operating and management index.

Furthermore, a time of H_2 cost parity, which occurs because unit H_2 production cost from PEM water electrolysis using electricity generated from renewable energy sources is less than or same as the one from conventional fossil fuel-based H_2 production such as natural gas steam reforming (grey H_2 production cost), should be estimated to realize green H_2 production method in commercial level, through techno-economic analysis. In particular, unit grey H_2 production cost by 2050 was estimated corresponding to the relationship with natural gas price (Equation 16) [10], because grey H_2 production cost depends on natural gas price and natural gas price.

$$H_2 \text{ cost } [\$\ \text{kg}^{-1}] = (0.217 \times \text{Natural gas price } [\$\ \text{GJ}^{-1}] + 0.15) \times \text{inflation} \tag{16}$$

, where inflation rate is 1.46% (i.e., 1 \$ in 2002 is worth 1.4 \$ in 2018).

Fig. 23 shows the expected grey H_2 production cost (without carbon capture and storage technology) by 2050, corresponding to the expected natural gas [11].

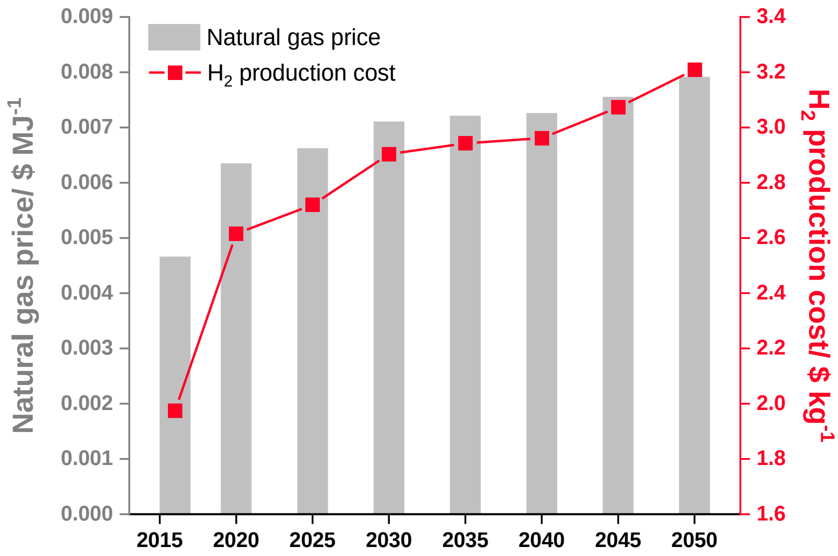


Fig. 23. Expected grey H_2 production cost by 2050 corresponding to the natural gas price.

Therefore, the time of H_2 cost parity was identified based on our results and the expected grey H_2 production cost through the economic parity analysis.

2.2.4. Sensitivity analysis

Sensitivity analysis is widely used to analyze how the target variable is affected based on the changes in input variables under uncertainty. In particular, this work was performed to quantify the effect of the changes in some input variables such as LCOE, system efficiency (based on higher heating value, HHV), current density, and maintenance ratio, on unit H_2 production cost, and to determine the input variable to be the most affected. From sensitivity analysis results, it can provide economic insight on what research fields will be concentrated on to make new or promising technology cost-competitive compared to conventional and fossil fuel-based processes. Table 3 lists items and values of input variables for green H_2 production by PEM water electrolysis using renewable energy-based electricity.

Table 3 Input variables for sensitivity analysis

Item	Minimum	Median	Maximum
Electricity price	-50%	0%	30%
System efficiency (based on HHV)	43%	53%	70.36%
Current density	1.5 A cm^{-2}	1.7 A cm^{-2}	3.0 A cm^{-2}
Maintenance ratio	1.5%	4%	10%

Reference

[1] NREL, Manufacturing cost analysis for proton exchange membrane water electrolyzer (2019).

[2] Turton R, Bailie RC, Whiting WB, Shaeiwitz JA, Bhattacharyya D. Analysis,

synthesis, and design of chemical processes. 4th ed. New Jersey: Pearson; 2013.

[3] O. Schmidt, A. Gambhir, I. Staffell, A. Hawkes, J. Nelson, S. Few, "Future cost and performance of water electrolysis: An expert elicitation study.", International Journal of Hydrogen Energy 42 (2017) 30470-30492.

[4] S. Deng, X. Guan, J. Xu, "The coopetition effect of learning-by-doing in outsourcing.", International Journal of Production Research (2019) 1-26.

[5] Pierre-Etienne FRANC, At the heart of the energy transition, Air Liquid (2020).

[6] W. Kuckshinrichs, T. Ketelaer, J. C. Koj, Economic analysis of improved alkaline water electrolysis. Frontiers in Energy Research 5 (2017) 1.

[7] B. P. Center, "Annual Energy Outlook 2020.", Energy Information Administration, Washington, DC (2020).

[8] Renewable Capacity Statistics 2020, International Renewable Energy Agency; 2020 March.

[9] A. Buttler, H. Spliethoff, Current status of water electrolysis for energy storage, grid balancing and sector coupling via power-to-gas and power-to-liquids: A review. Renewable and Sustainable Energy Reviews 82 (2018) 2440-2454.

[10] B. Parkinson, P. Balcombe, J.F. Speirs, A.D. Hawkes, K. Hellgardt, Levelized cost of CO_2 mitigation from hydrogen production routes. Energy & Environmental Science 12 (2019) 19.

[11] A. Sieminski, Annual Energy Outlook 2017, U.S. Energy Information Administration (2017).

3. Life cycle assessment

Life cycle assessment is a useful tool to evaluate environmental impacts by considering all inputs and outputs along with the entire green H_2 production by PEM water electrolysis using electricity generated from renewable energy sources, in terms of holistic perspective complying with International Organization for Standardization (ISO). In general, there are four steps to conduct life cycle assessment according to the ISO standard; 1) goal and scope definition, 2) life cycle inventory analysis, 3) life cycle impact assessment and 4) interpretation, as shown in Fig. 24 [1].

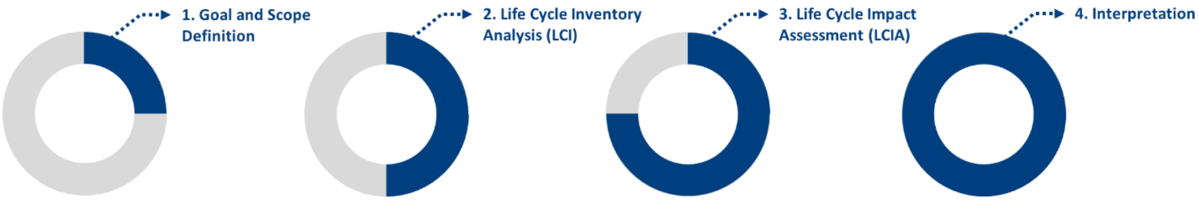


Fig. 24. 4 steps of a life cycle assessment

The first is to define the goal and scope of this work and this step is the most important because important LCA elements such as a system boundary, a functional unit, and cut-off, affecting results in other steps, were determined. Here, a system boundary is of utmost importance for life cycle assessment and classified into four types; cradle-to-grave, cradle-to-gate, gate-to-gate, and gate-grave. In this work, cradle-to-gate system boundary including the processes from raw material extraction to the production phase (i.e. all processes before use of the product), was chosen for green H_2 production by PEM water electrolysis using electricity generated from renewable energy sources and gate-to grave system for all downstream processes after manufacturing was excluded due to the same product (H_2) in this work and the extensive H_2 utilization fields such as ammonia production, chemical industry/refineries, electronic industry, metal/glass industry, H_2 refueling station, and fuel cell, as shown in Fig. 25 [2].

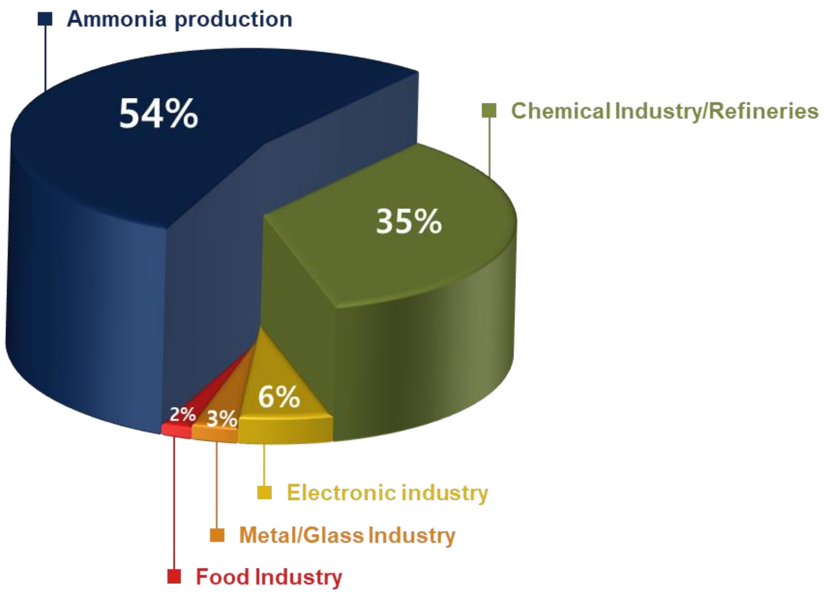


Fig. 25. Distribution of a global H_2 market

In addition, 1 kg of H_2 production by PEM water electrolysis system was decided as a functional unit and 0.1% cut off was set to show the filtered data. The second is life cycle inventory analysis to gather material input and output data for green H_2 production by PEM water electrolysis system and environmental impact data through Ecoinvent 3 database, by employing SimaPro, which is one of the powerful software tools for life cycle assessment. Here, using commercial software is recommended because it makes life cycle inventory analysis facilitate and help to collect a lot of data required for obtaining the accurate life cycle assessment results. Table 4 shows all input data to build a PEM water electrolysis system [3] using electricity generated from each renewable energy source such as solar PV, onshore wind, and hydropower.

Table 4 All input data for 1 kg of green H_2 production by PEM water electrolysis system using electricity generated from different renewable energy sources

Item	Material	
PEM water electrolysis stack	Titanium, primary (GLO)	528 kg
	Aluminum, primary, ingot (RoW)	27 kg
	Stainless steel, Scarp	100 kg
	Copper, primary (RER)	4.5 kg

	Tetrafluoroethylene, market (GLO)	16 kg
	Iridium, from nature	0.75 kg
	Platinum, market (GLO)	0.075 kg
	Activated carbon, granular (GLO)	9 kg
Balance of plant	Steel, low-alloyed (RER)	6.7 ton
	Concrete, normal (CH)	2.33 m^3
	Polyethylene, high density (GLO)	0.3 kg
	Copper, primary (RER)	0.05 kg
	Aluminum, primary (RoW)	0.05 kg
	Electronics, control units (GLO)	1.1 kg
Gas purification	Silica sand, market (GLO)	1 kg
	Electricity, natural gas, conventional power plant (KR)	0.05 kWh
Electricity	(a) Electricity, natural gas, conventional power plant (KR)	73.93 kWh kg^{-1} (current) 60.1 kWh kg^{-1} (future)
	(b) Electricity, photovoltaic, open ground installation (KR)	
	(c) Electricity, wind, turbine, onshore (KR)	
	(d) Electricity, hydro, pumped storage (KR)	

**GLO: Global, RoW: Rest-of-World, RER: Europe without Germany, the Netherlands, and Russia, CH: Switzerland, and KR: Republic of Korea

The third is life cycle impact assessment to translate the collected inventory data in step 2 into the selected environmental impacts by considering characterization factors based on each environmental impact category. For life cycle impact assessment, there are two pathways to derive characterization factors; midpoint and endpoint indicators. Here, the midpoint indicator focuses on each environmental issue such as global climate change caused by global warming, ozone depletion, and particular matter formation whereas the endpoint indicator concentrates on 3 aggregation levels; Damage to 1) human health, 2) ecosystems and 3) resource availability [4]. In this work, ReCipe 2016 Midpoint (Hierarchy version) method was used because midpoint level is easier to obtain lower uncertain LCA results than endpoint level [5]. Table 5 describes the environmental impact categories covered in this work.

Table 5 Description of the considered environmental impact categories for LCA

Impact category	Unit	Description
Global warming	kg CO_2 eq.	• Indicator of potential global warming because of greenhouse gases emission to the atmosphere. • Contribution to global climate change.
Ozone depletion	kg CFC11 eq.	• Indicator of potential ozone depletion due to the emission of chemicals containing gaseous chlorine or bromine to the atmosphere. • Contribution to ozone layer depletion.
Fine particular matter formation	Kg PM2.5eq.	• Indicator of potential fine particular matter formation owing to the SO_2, NO_x, NH_3, CO, and volatile organic compounds to the atmosphere. • Contribution to human disease burden.

In particular, global warming, ozone depletion, fine particular matter formation are selected as environmental impact categories because three impacts are quality level I, recommendations by Joint Research Centre [6]. Last is interpretation to summarize results of life cycle inventory analysis and life cycle inventory analysis. Furthermore, the results of environmental impact per functional unit considering each characterization factor can be obtained for green H_2 production by PEM WE system using each renewable energy-based electricity.

Reference

[1] N. von der Assen, P. Voll, M. Peters, A. Bardow, Life cycle assessment of CO_2 capture and utilization: a tutorial review. Chemical Society Reviews 43 (2014) 7982.

[2] B. Lee, H. Lim, Cost-competitive methane steam reforming in a membrane reactor for H_2 production: Technical and economic evaluation with a window of a H_2 selectivity. International Journal of Energy Research 43 (2019) 1468-1478.

[3] K. Bareiß, C. de la Rua, M. Möckl, T. Hamacher, Life cycle assessment of hydrogen production from proton exchange membrane water electrolysis in future energy systems, *Applied Energy* 237 (2019) 862-872.

[4] J. C. Bare, P. Hofstetter, D. W. Pennington, H. A. U. de Haes, Midpoints versus endpoints: The sacrifices and benefits, International Journal of Life Cycle Assessment 5 (2000) 319-326.

[5] M. A. J. Huijbregts, Z. J. N. Steinmann, P. M. F. Elshout, G. Stam, F. Verones, M. Vieira, M. Zijp, A. Hollander, R. van Zelm , ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level, International Journal of Life Cycle Assessment 22 (2017) 138-147.

[6] Annual Energy Outlook 2017, EIA (2017).

4. Analytic hierarchy process

An analytic hierarchy process developed by Thomass L. Saaty [1], is one of the most commonly used multi-criteria decision analysis methods to investigate and analyze complex decisions owing to a lot of criteria [2]. The ultimate goal of the analytical hierarchy process is to calculate the priorities of each alternative based on rigorous assessment results on the weighted values for each criterion, compare alternatives based on criteria with different weighted points, and therefore help decision-makers determine the best alternative effectively based on multiple evaluation criteria. There are five steps to conduct the analytic hierarchy process 1) present alternatives, 2) define criteria influencing the selection of the best alternative, 3) conduct pair-wise comparisons, in sequence, 4) calculate priorities of each alternative with the different weighted points of criteria, and 5) make a decision for the best alternative (i.e., renewable energy source) of green H_2 production by PEM WE system. Here, a pairwise comparison matrix was created through Equation 17–21.

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} \tag{17}$$

$$a_{ij} = \frac{a_i}{a_j} \ (i, j = 1, \cdots, n) \tag{18}$$

$$\bar{A} = \begin{bmatrix} \bar{a}_{11} & \cdots & \bar{a}_{1n} \\ \vdots & \ddots & \vdots \\ \bar{a}_{n1} & \cdots & \bar{a}_{nn} \end{bmatrix} \tag{19}$$

$$\bar{a}_{ij} = \frac{a_i}{\sum_i^n a_{ij}} \ (i, j = 1, \cdots, n) \tag{20}$$

$$p_i = \frac{\sum_j^n \bar{a}_{ij}}{\sum_i \sum_j \bar{a}_{ij}} \tag{21}$$

, where a_i and a_j are results corresponding on each criterion, and $\bar{a}_{ij}$ is normalized one by dividing the sum of column for matrix A. For pair-wise comparison, a matrix for each criterion was built and priority (p_i) was calculated to set priorities.

The first hierarchy was built for techno-economic and environmental criteria, based on unit H_2 production cost and CO_2 emission for global warming, respectively, at the current and future level. In addition, a total weighted value of 1 was assumed: for example, the weighted value for environmental criterion is 5, if one for techno-economic criterion is 5. Table 6–7 present the pair-wise comparison matrix results with the weighted values for techno-economic and environmental criteria of 5 and 5, at the current and future levels.

Table 6 Pair-wise comparison matrix with the weighted values for techno-economic and environmental criteria of 5 and 5, in the current level

	Techno-economic	**Environmental**	**Priority**
Solar PV	0.1276	0.1543	**0.2819**
Onshore wind	0.1779	0.3282	**0.5061**
Hydropower	0.1946	0.0175	**0.2121**

Table 7 Pair-wise comparison matrix with the weighted values for techno-economic and environmental criteria of 5 and 5, in future level

	Techno-economic	**Environmental**	**Priority**
Solar PV	0.2160	0.1602	**0.3762**
Onshore wind	0.1714	0.3207	**0.4920**
Hydropower	0.1127	0.0191	**0.1318**

Here, higher priority means a more appropriate alternative for green H_2 production in terms of techno-economic and environmental perspectives, simultaneously. Therefore, solar PV, onshore wind, and hydropower were considered as alternatives, and unit H_2 production cost (for techno-economic criteria) and CO_2 emission for global warming (for environmental criteria) were taken into account of sub-criteria, with different weighted values of criteria under determination or uncertainty, to find the most appropriate renewable energy source for green H_2 production by PEM water electrolysis.

Reference

[1] T. L. Satty, What is the analytic hierarchy process?, Mathematical models for decision support, Springer, Berlin, Heidelberg 1988.

[2] S. Zhou, P. Yang, Risk management in distributed wind energy implementing analytic hierarchy process, Renewable Energy 150 (2020) 616-623.

5. Results and discussion

5.1. Process simulation

Fig. 26 shows the process flow diagram of PEM water electrolysis for green H_2 production based on some electrochemical parameters and the effect of current density and cell active area on H_2 production rate was confirmed as shown in Fig. 27.

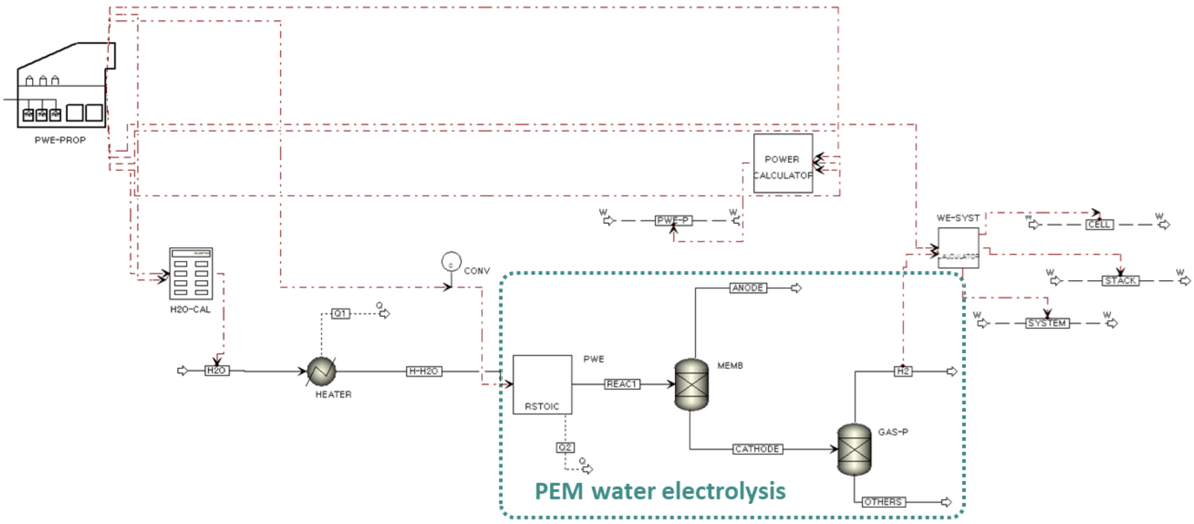


Fig. 26. Process flow diagram of PEM water electrolysis for green H_2 production

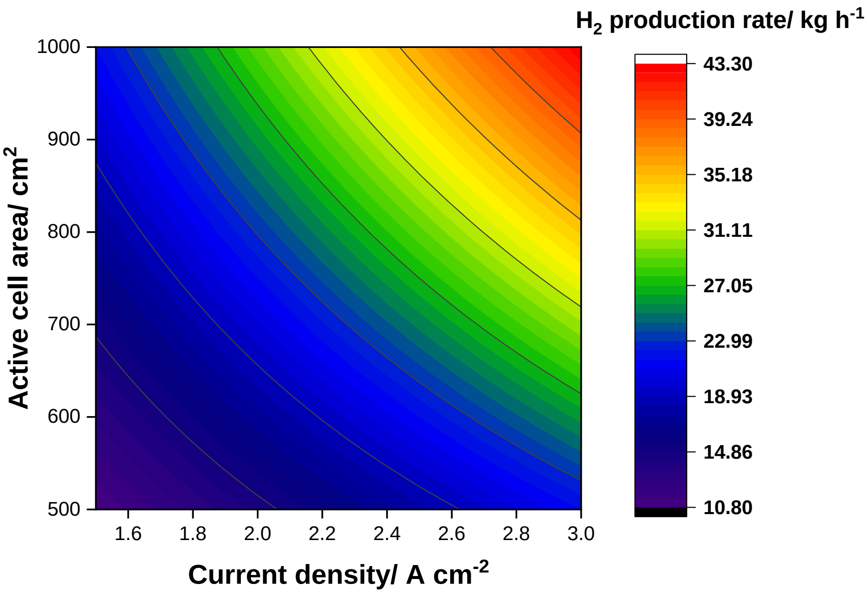


Fig. 27. Effect of current density and active cell area on H_2 production rates

First of all, it can be clearly shown that current density has greater influences on H_2 production rates than active cell area, indicating that higher current density, as well as cell active area, can make unit H_2 production cost lower and feasible. Based on process simulation results, functional specifications of PEM water electrolysis system in current and future level for 10 MW capacity were considered to conduct economic analysis as shown in Table 8.

Table 8 Functional specifications of the PEM water electrolysis system

	Current level	**Future level**	**Unit**
Faradaic efficiency	75.8	80.2	%
Current density	1.7	3.0	A cm^{-2}
Potential	2.1	1.8	V
Cell active area	680	1,000	cm^{-2}
Cell #	510		
Power density	3.55	2.89	W cm^{-2}
Required energy	6.6	5.4	kWh Nm^{-3}
Efficiency (HHV)	45.04	55.36	%
Efficiency (LHV)	53.29	65.52	%
H_2 yield	17.5	22.0	kg h^{-1}
Durability	7	10	years
Experience rate	-	18	%
Stream factor	0.93		

*Low heating value (LHV)

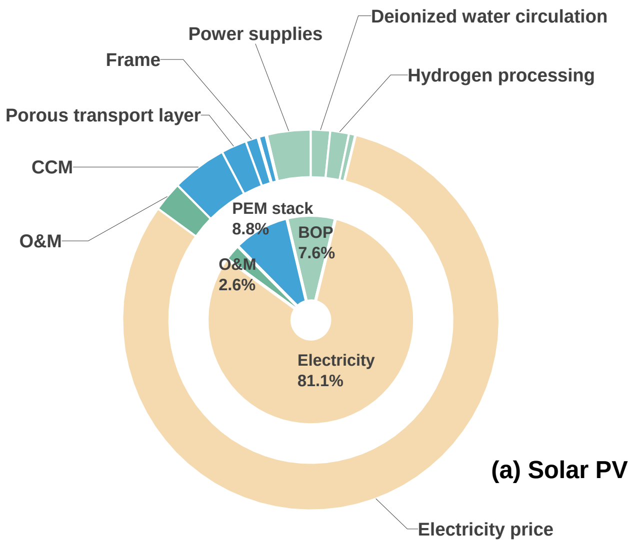
5.2. Economic analysis

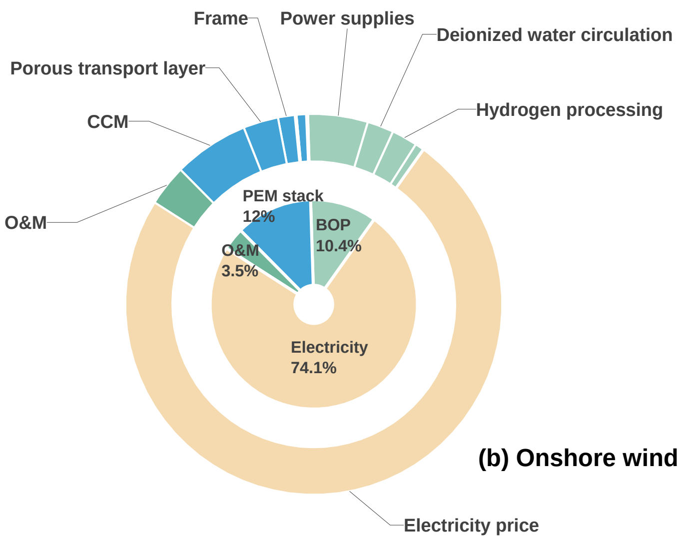
Table 9 shows itemized cost estimation for green H_2 production (10 MW capacity) with different LCOEs according to the different renewable energy sources such as solar PV, onshore wind, and hydropower.

Table 9 Itemized cost estimation for green H_2 production by PEM water electrolysis system with solar PV, onshore wind, and hydropower-based electricity in the current level

	Solar PV/\$ kgH_2^{-1}	Onshore wind/\$ kgH_2^{-1}	Hydropower/\$ kgH_2^{-1}
Capital cost	**0.940**	**0.940**	**0.940**
CCM	0.359	0.359	0.359
Porous transport layer	0.168	0.168	0.168
Frame	0.080	0.080	0.080
Biopolar plates	0.009	0.009	0.009
Assembly & End-plates	0.045	0.045	0.045
Balance of stack	0.009	0.009	0.009
Power supplies	0.285	0.285	0.285
Deionized water circulation	0.127	0.127	0.127
Hydrogen processing	0.123	0.123	0.123
Cooling	0.041	0.041	0.041
Miscellaneous	0.004	0.004	0.004
Operating cost	**6.209**	**4.133**	**3.681**
Electricity price	6.279	4.180	3.722
O&M	1.605	1.605	1.605
Total cost	**7.345**	**5.268**	**4.816**

From Table 8, respective unit H_2 production costs of 7.345, 5.268, and 4.816 \$ kgH_2^{-1} for green H_2 production by PEM water electrolysis using solar PV, onshore wind, and hydropower, respectively, were obtained showing that green H_2 production cost has approximately 2–4 times higher than one from grey H_2 production of under 2 \$ kgH_2^{-1} (i.e., methane steam reforming without carbon capture and storage technology) [1]. In addition, Fig. 28 presents the percentage distribution of items to unit H_2 production cost with different renewable energy sources-based electricity.


Deionized water circulation
Power supplies
Frame
Hydrogen processing
Porous transport layer
CCM
O&M
PEM stack
8.8%
BOP
7.6%
O&M
2.6%
Electricity
81.1%
(a) Solar PV
Electricity price


Frame
Power supplies
Deionized water circulation
Porous transport layer
Hydrogen processing
CCM
O&M
PEM stack
12%
BOP
10.4%
O&M
3.5%
Electricity
74.1%
(b) Onshore wind
Electricity price

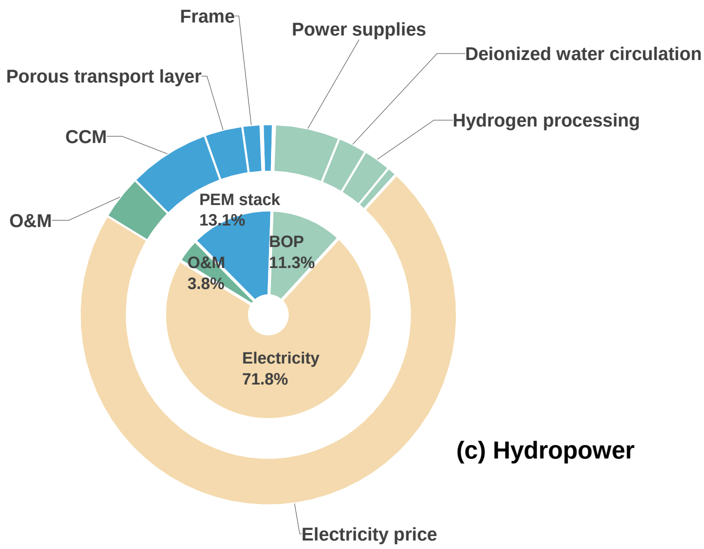
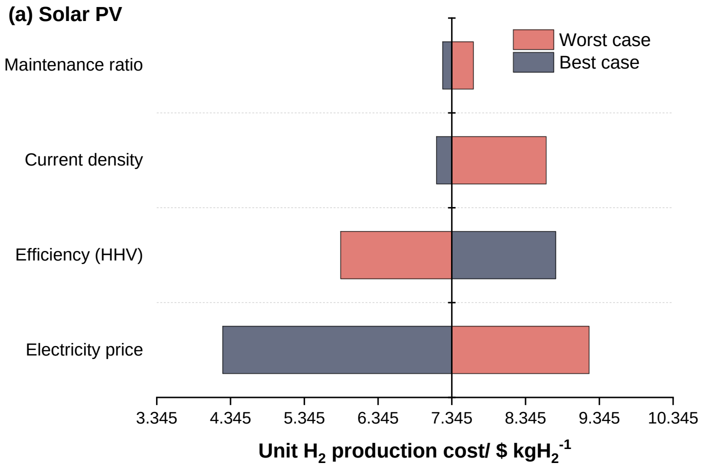
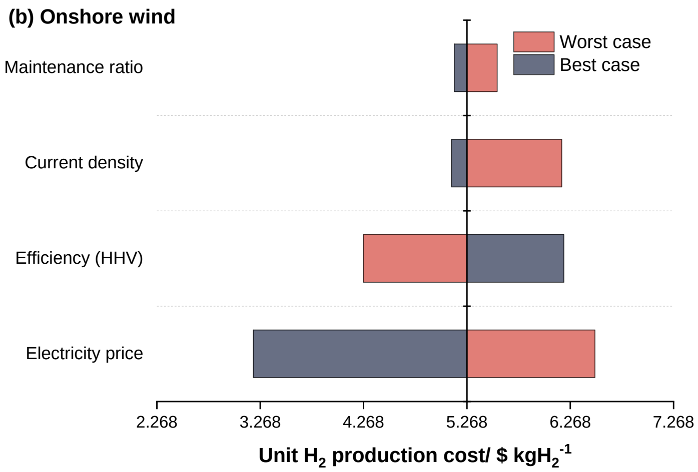


Fig. 28. The percentage distribution of items to unit H_2 production cost by PEM water electrolysis for green H_2 production with electricity generated from (a) solar PV, (b) onshore wind, and (c) hydropower.

From Fig 28, the percentage of electricity price to unit H_2 production cost is 84.5%, 78.4%, and 76.4% for solar PV, onshore wind, and hydropower, respectively, while the respective ratios of PEM water electrolysis system price to the unit H_2 production cost of 12.8%, 17.8%, and 19.5% are obtained. The point that electricity price accounts for approximately 70–80% of unit H_2 production cost is general and these results are reasonable according to the previously reported paper [2]. Moreover, solar PV based-electricity price is higher than others in current level and lower unit H_2 production cost should be necessary to make green H_2 production technology cost-competitive compared to one from conventional H_2 production cost, by taking into account how to reduce the unit H_2 production cost in terms of capital and operating costs. Furthermore, Fig. 29 presents sensitivity analysis results on unit H_2 production cost with the changes of values for input variables.


(a) Solar PV
Worst case
Best case
Maintenance ratio
Current density
Efficiency (HHV)
Electricity price
3.345
4.345
5.345
6.345
7.345
8.345
9.345
10.345
Unit H_2 production cost/ $ kgH_2^{-1}


(b) Onshore wind
Worst case
Best case
Maintenance ratio
Current density
Efficiency (HHV)
Electricity price
2.268
3.268
4.268
5.268
6.268
7.268
Unit H_2 production cost/ $ kgH_2^{-1}

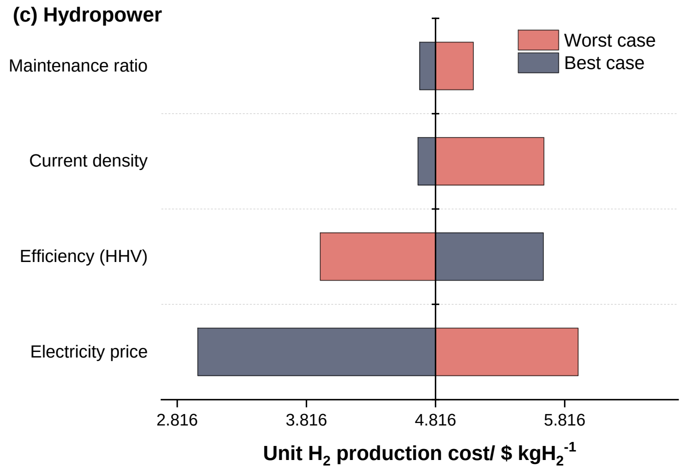
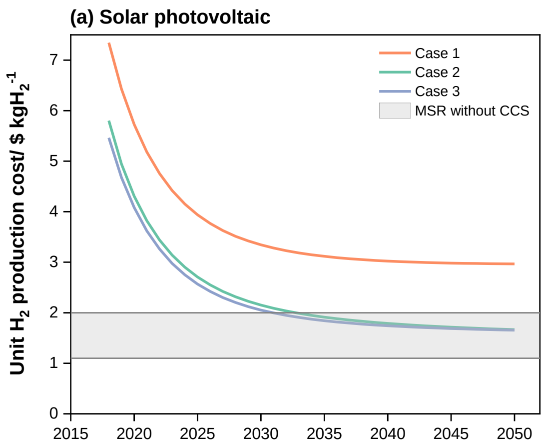
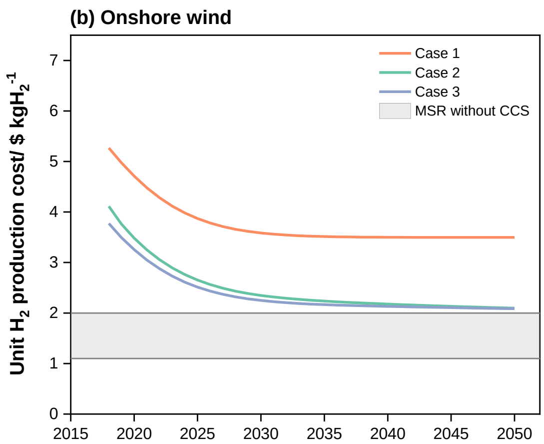


Fig. 29. Sensitivity analysis results on unit H_2 production cost by PEM water electrolysis for green H_2 production with electricity generated from (a) solar PV, (b) onshore wind, and (c) hydropower.

From sensitivity analysis results, electricity price is the most affecting economic parameter on unit H_2 production cost for all cases covered in this work. However, only changing one economic parameter should not make green H_2 production by PEM water electrolysis using renewable energy-based electricity attractive and feasible. Therefore, capital cost reduction through scale-up, technology development, and experience rate, which can result in the cost reduction of manufacture owing to the accumulated production experience, as well as electricity price should be decreased by considering LCOE reduction resulting in the increasing renewable energy capacity (Fig. 21). In this work, methods of capital cost reduction are divided into four cases: Case 1 is the base case for 10 MW PEM water electrolysis system with some functional specifications at the current level, as presented in Table 8, Case 2 is the advanced case for 10 MW PEM water electrolysis system with some functional specifications in future level, and Case 3 is the advanced case for 1,000 MW PEM water electrolysis system. Here, all cases considered an experience rate of 18%. Figs. 30–33 present economic forecast analysis results of green H_2 production by PEM water electrolysis using electricity generated from different renewable energy sources, if the percentage of green H_2 production among global H_2 are different, based on the expected LCOE and global H_2 demand that is done.


(a) Solar photovoltaic
Case 1
Case 2
Case 3
MSR without CCS
Unit H_2 production cost/ \$ kgH_2^{-1}
0
1
2
3
4
5
6
7
2015
2020
2025
2030
2035
2040
2045
2050


(b) Onshore wind
Case 1
Case 2
Case 3
MSR without CCS
Unit H_2 production cost/ \$ kgH_2^{-1}
0
1
2
3
4
5
6
7
2015
2020
2025
2030
2035
2040
2045
2050

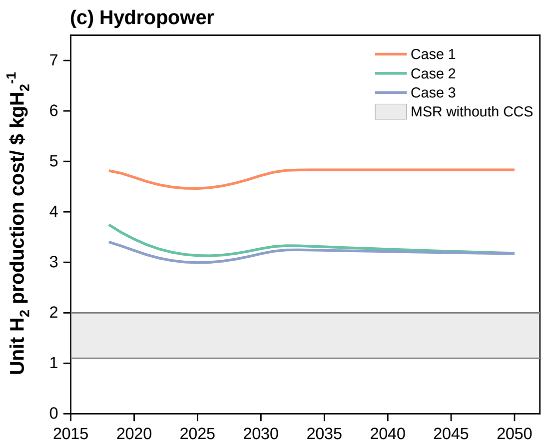
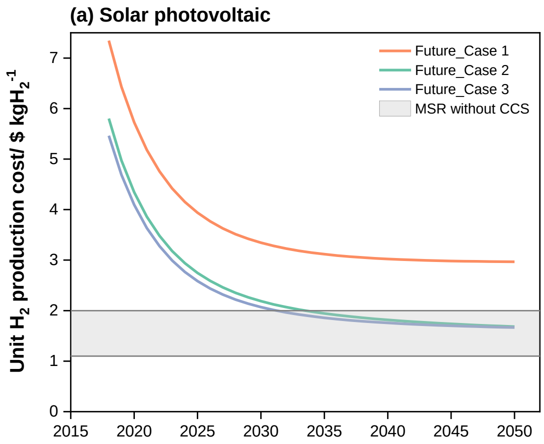
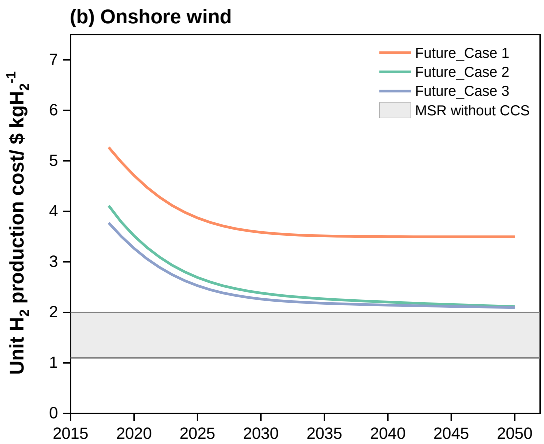

(c) Hydropower
Case 1
Case 2
Case 3
MSR withouth CCS
Unit H_2 production cost/ \$ kgH_2^{-1}
0
1
2
3
4
5
6
7
2015
2020
2025
2030
2035
2040
2045
2050

Fig. 30. Economic forecast analysis of green H_2 production using electricity generated from (a) solar PV, (b) onshore wind, and (c) hydropower with 100% of H_2 production from water electrolysis.





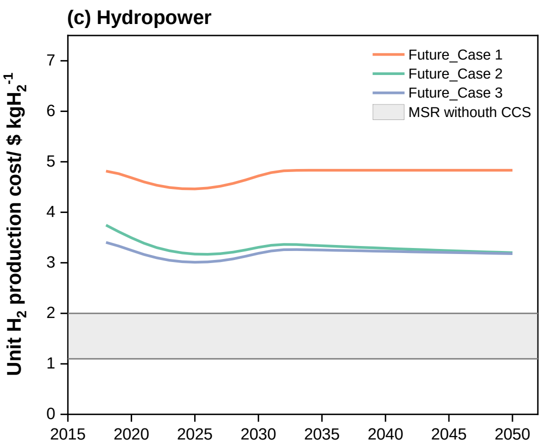
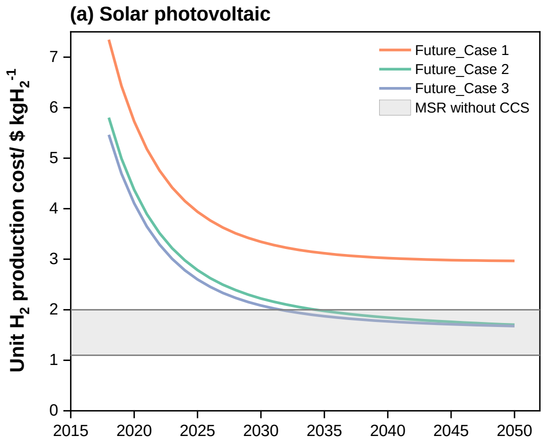
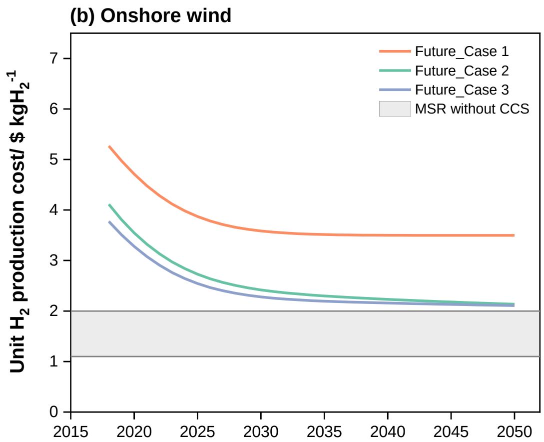


Fig. 31. Economic forecast analysis of green H_2 production using electricity generated from (a) solar PV, (b) onshore wind, and (c) hydropower with 70% of H_2 production from water electrolysis.


(a) Solar photovoltaic
Unit H2 production cost/ $ kgH2-1
Future_Case 1
Future_Case 2
Future_Case 3
MSR without CCS
0
1
2
3
4
5
6
7
2015
2020
2025
2030
2035
2040
2045
2050


(b) Onshore wind
Unit H2 production cost/ $ kgH2-1
Future_Case 1
Future_Case 2
Future_Case 3
MSR without CCS
0
1
2
3
4
5
6
7
2015
2020
2025
2030
2035
2040
2045
2050

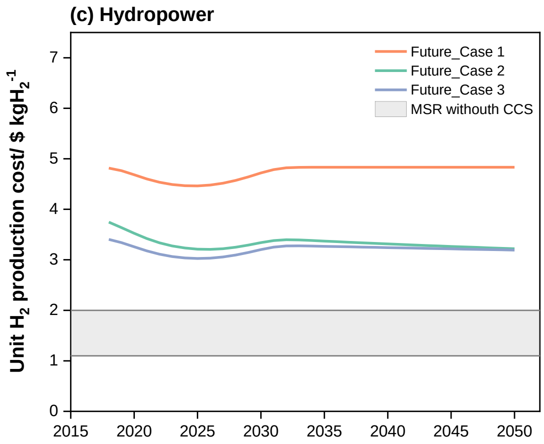
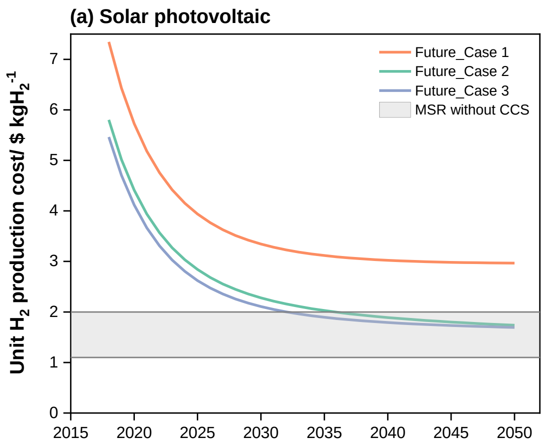


Fig. 32. Economic forecast analysis of green H_2 production using electricity generated from (a) solar PV, (b) onshore wind, and (c) hydropower with 50% of H_2 production from water electrolysis.



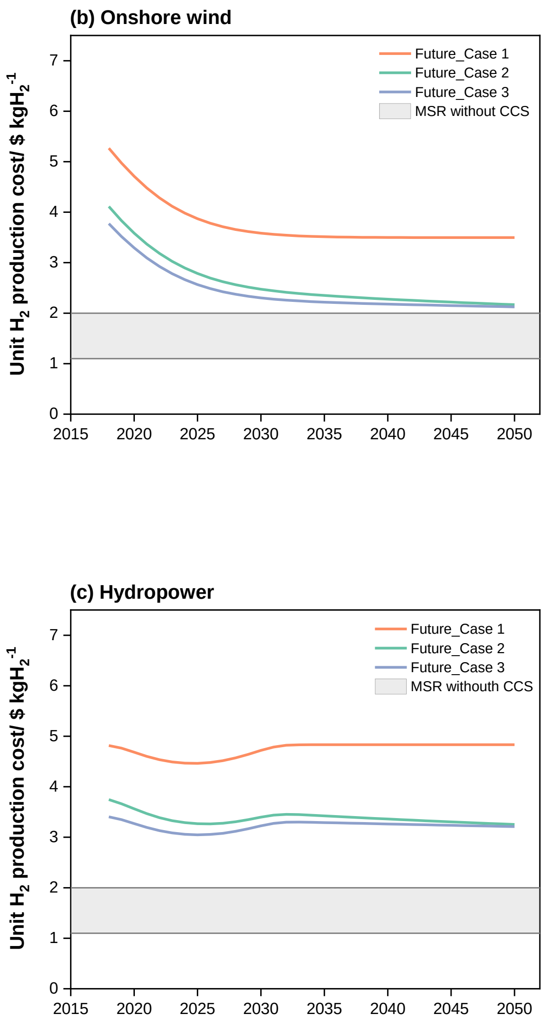


Fig. 33. Economic forecast analysis of green H_2 production using electricity generated from (a) solar PV, (b) onshore wind, and (c) hydropower with 30% of H_2 production from water electrolysis.

First of all, the percentage of green H_2 production among global H_2 production has little impact on unit H_2 production cost, because PEM water electrolysis system price accounts for approximately 20% of unit H_2 production cost. It means that PEM water electrolysis system cost reduction has little impact on unit H_2 production cost compared to electricity price reduction. From Fig. 30, it can be clearly shown that cases 2 and 3 for green H_2 production by PEM water electrolysis using solar PV-based electricity were only feasible compared to green H_2 reached grey H_2 production cost by MSR with carbon capture and storage (less than 2 \$ kgH_2^{-1}) and approximately 2032 and 2034 green H_2 reached grey H_2 production cost. It is because lower LCOE is caused by the increase in solar PV energy capacity, compared to others. And, Table 10 listed reaching time to be equal to or less than green H_2 production cost compared to grey H_2 production cost, for cases using solar PV.

Table 10 Reaching time to be equal or less than green H_2 production cost compared to < 2 \$ kgH_2^{-1}

	*Solar PV_100%	*Solar PV_70%	*Solar PV_50%	*Solar PV_30%
Case 1	-	-	-	-
Case 2	2033	2034	2035	2036
Case 3	2031	2032	2032	2033

*Here, Solar PV_100% means the case is green H_2 production by PEM water electrolysis using electricity generated from solar PV with 100% green H_2 production among global H_2 demand.

In particular, it seems that green H_2 production can be feasible compared to grey H_2 production after 2030. This is because of the decrease in LCOE resulting in the dramatic increase in solar PV energy capacity by 2030, the advanced PEM water electrolysis technology, and scale-up, thanks to many countries have made a lot of effort to address environmental issues, especially global warming.

Moreover, the interesting thing from these results is hydropower should not be utilized for electricity generation sources due to the disadvantages of hydropower, such as carbon and methane emission, the effect of water quality and flow, the prospect of low dissolved oxygen levels in the water, the destruction of wildlife habitat, to name a few, although hydropower is the most important and widely used renewable energy source due to the lower LCOE among renewable energy sources, the relatively mature technology, and so on, in the current level. Furthermore, green H_2 production using onshore wind-based electricity has the possibility to be cost-competitive compared to one from grey H_2 production, if onshore wind energy capacity has been significantly increasing.

In addition, economic parity analysis of green H_2 production by PEM water electrolysis using electricity generated from solar PV with 100% of H_2 production from water electrolysis was carried out and Fig. 34 shows economic parity analysis results based on the increase in grey H_2 production cost caused by the increase in natural gas price.

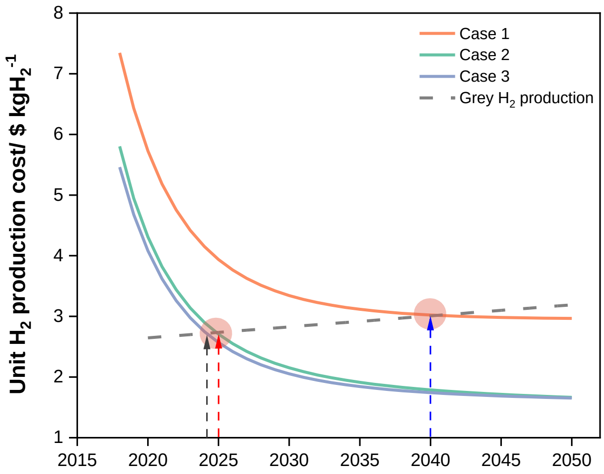
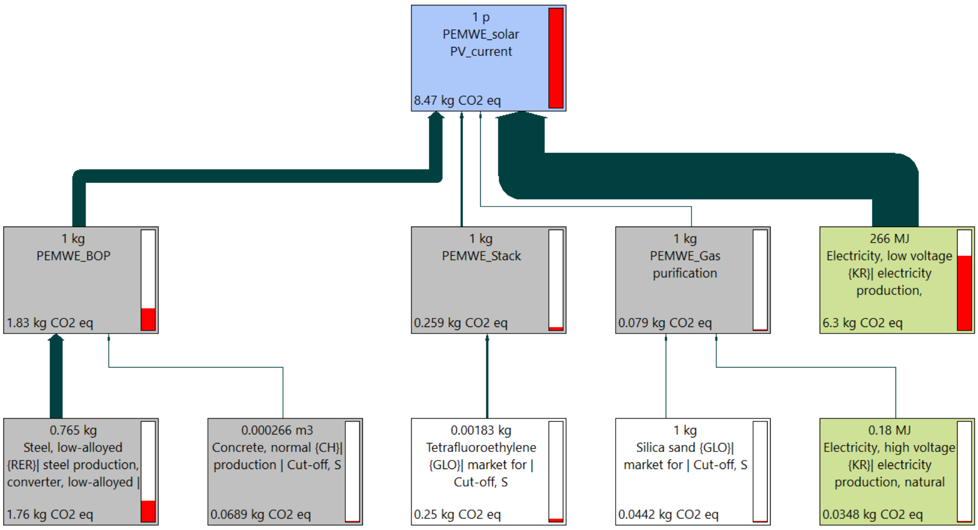


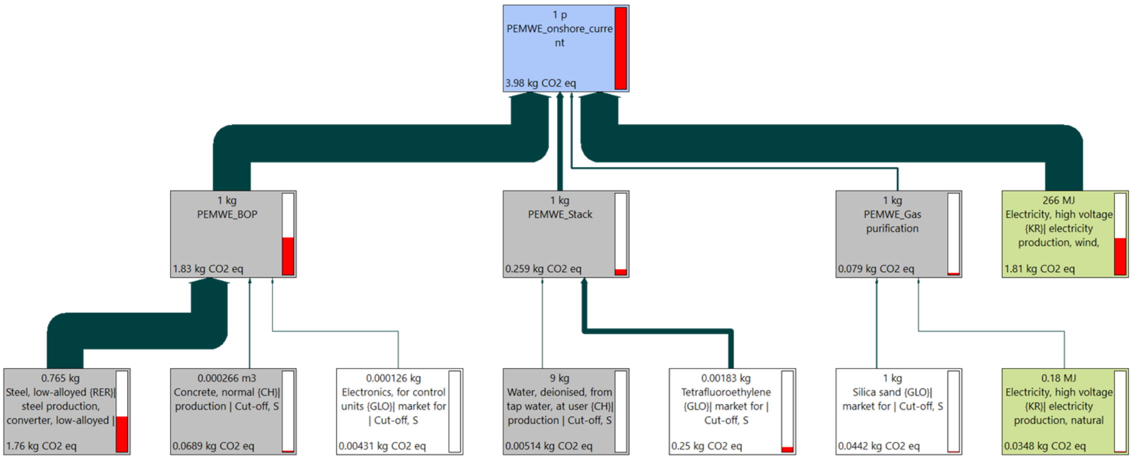
Fig. 34. Economic parity analysis of green H_2 production using electricity generated from solar PV based on the expected grey H_2 production cost.

From Fig. 34, around 2040 H_2 parity will be reached when the level of PEM water electrolysis system technology is at the current level, because of lower LCOE compared to now, although PEM water electrolysis system cost and the required energy are higher. On the other hand, H_2 parity can occur in approximately 2025 and 2024, for cases 2 and 3, respectively, if PEM water electrolysis system technology is developed by future level, covered in this work. From these results, green H_2 production by PEM water electrolysis using electricity generated from solar PV is a promising technology in terms of the economic perspective. Therefore, it can be figured out that green H_2 will be fully utilized as the promising energy carrier in the future, in terms of the economic aspect, if the technology of the PEM water electrolysis system is developed as well as LCOE is lower owing to the increase in the installed renewable energy capacity and provide economic insights to assist decision-making (such as the government policy direction on "Hydrogen Economy").

5.3. Life cycle assessment

Fig. 35–36 present life cycle assessment results by using Sankey diagram to identify the entire life cycle environmental impact for green H_2 production by PEM water electrolysis using electricity generated from different renewable energy sources at the current level and future level, respectively, in terms of CO_2 emission, and find out the hot-spot, which has a decisive effect on environmental impacts for the overall system. Moreover, Table 11–13 tabulate environmental impact assessment results for each unit, in detail, in terms of CO_2 emission, ozone depletion, and fine particular matter formation, respectively.





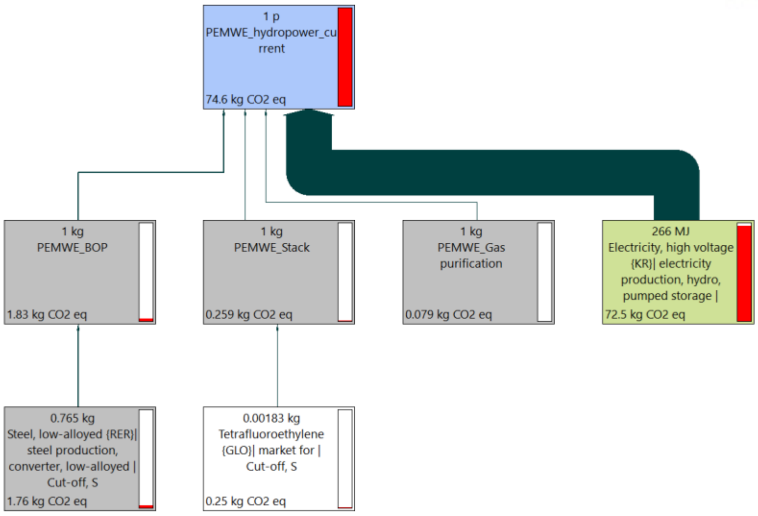
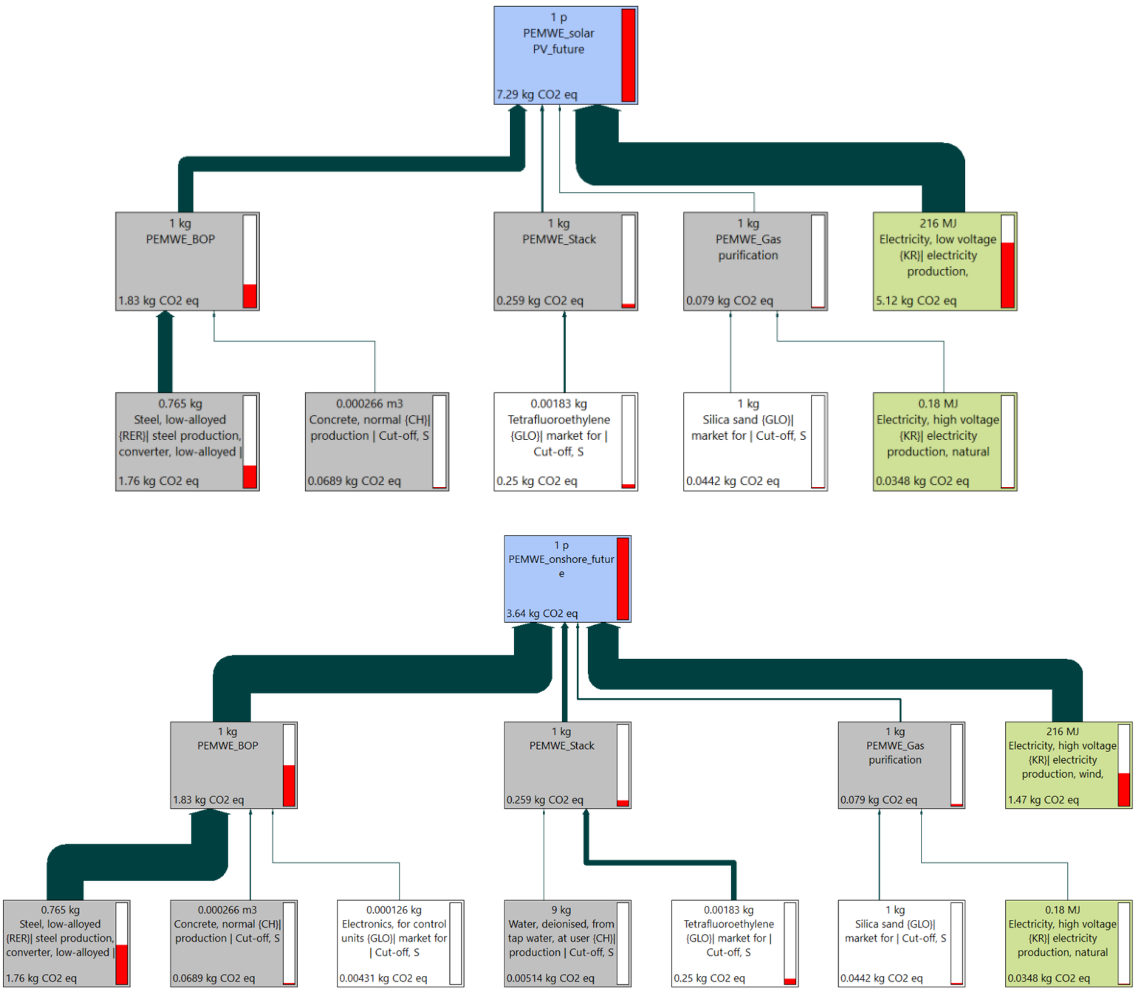


Fig. 35. Environmental impact of CO_2 emission for green H_2 production, in order of solar PV, onshore wind, and hydropower, in the current level.



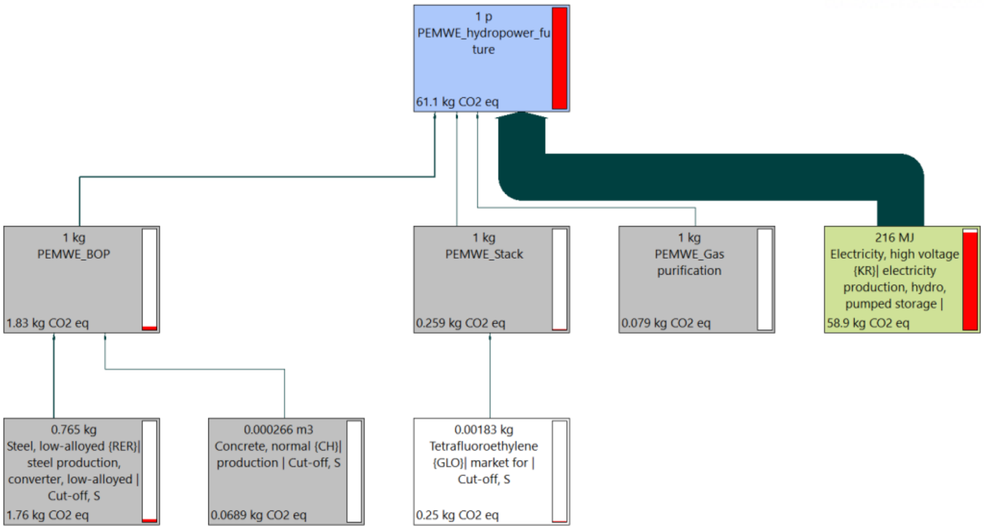


Fig. 36. Environmental impact of CO_2 emission for green H_2 production, in order of solar PV, onshore wind, and hydropower, in future level.

Table 11 Environmental impact of CO_2 emission of each unit for green H_2 production using different electricity generation sources (solar PV, onshore wind, and hydropower)

	Electricity generation source	**Unit. kgCO$_2$-eq.**			
		PEM water electrolysis stack	Balance of plant	Gas purification	Electricity
Current level	Solar PV	0.259	1.834	0.079	6.299
	Onshore wind	0.259	1.834	0.079	1.810
	Hydropower	0.259	1.834	0.079	72.477
Future level	Solar PV	0.259	1.834	0.079	5.121
	Onshore wind	0.259	1.834	0.079	1.472
	Hydropower	0.259	1.834	0.079	58.919

Table 12 Environmental impact of ozone depletion of each unit for green H_2 production using different electricity generation sources (solar PV, onshore wind, and hydropower)

	Electricity generation source	**Unit/ kgNO$_x$-eq.**			
		PEM water	Balance of	Gas	Electricity

		electrolysis stack	plant	purification	
Current level	Solar PV	0.00006	0.00544	0.00021	0.01675
	Onshore wind	0.00006	0.00544	0.00021	0.00623
	Hydropower	0.00006	0.00544	0.00021	0.16717
Future level	Solar PV	0.00006	0.00544	0.00021	0.01361
	Onshore wind	0.00006	0.00544	0.00021	0.00506
	Hydropower	0.00006	0.00544	0.00021	0.13590

Table 13 Environmental impact of find particular matter formation of each unit for green H_2 production using different electricity generation sources (solar PV, onshore wind, and hydropower)

	Electricity generation source	**Unit/ kgPM2.5 eq.**			
		PEM water electrolysis stack	Balance of plant	Gas purification	Electricity
Current level	Solar PV	0.00005	0.00468	0.00010	0.01410
	Onshore wind	0.00005	0.00468	0.00010	0.00628
	Hydropower	0.00005	0.00468	0.00010	0.08224
Future level	Solar PV	0.00005	0.00468	0.00010	0.01147
	Onshore wind	0.00005	0.00468	0.00010	0.00510
	Hydropower	0.00005	0.00468	0.00010	0.06686

Through environmental assessment results in terms of CO_2 emission, ozone depletion, and fine particular matter formation, the renewable energy source for electricity generation is the most important hot-spot affecting the life cycle environmental impact and the same orders of environmental impact (onshore wind, solar PV, and hydropower, from lowest to highest) was identified for all environmental impacts, covered in this work. In addition, respective CO_2 emissions of 8.471 kgCO_2-eq., 3.982 kgCO_2-eq., and 74.649 kgCO_2-eq. for solar PV, onshore wind, and hydropower, in current level of PEM water electrolysis system, were obtained and CO_2 emissions were 7.293 kgCO_2-eq., 3.644 kgCO_2-eq., and 61.091 kgCO_2-eq. for solar PV, onshore wind, and hydropower, respectively, in a future level of PEM water electrolysis system. From these results, the percentage decrease of CO_2

emissions caused by technology development of PEM water electrolysis system calculated 13.91%, 8.49%, and 18.16% for solar PV, onshore wind, and hydropower, respectively, based on Equation 22 indicating the lower energy requirement for 1 kg H_2 production from technology development of PEM water electrolysis system can lead to saving the use of electricity, resulting in lower unit H_2 production cost as well as CO_2 emission for 1 kg H_2 production.

$$Percentage\ decrease\ of\ CO_2\ emissions = \frac{(CO_{2,current} - CO_{2,future})}{CO_{2,current}} \times 100 \tag{22}$$

Moreover, CO_2 emission improvements calculated by Equation 23, were 28.82%, 66.54%, and -527.3% for solar PV, onshore wind, and hydropower in current level of PEM water electrolysis system and 38.71%, 69.38%, and -413.37% for solar PV, onshore wind, and hydropower in the current level, compared to CO_2 emission of 11.9 kgCO_2-eq. for 1 kg H_2 production from grey H_2 production [3], showing onshore wind > solar PV > hydropower in the order of higher CO_2 emission improvements for current and future level (Here, the CO_2 emission for grey H_2 production is considered as $CO_{2,ref.}$).

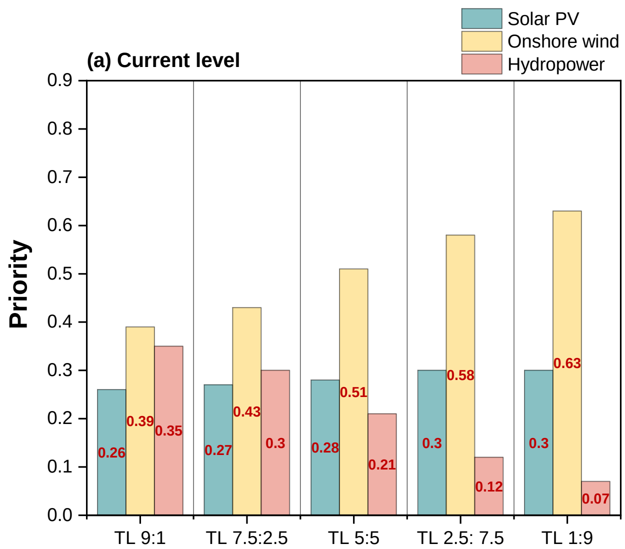
$$CO_2\ emission\ improvements = \frac{(CO_{2,ref} - CO_{2,i})}{CO_{2,ref}} \times 100 \tag{23}$$

From these results, hydropower has higher CO_2 emission compared to one emitted from conventional grey H_2 production and is not suitable if environmental aspect should be considered to determine the appropriate renewable energy source, although hydropower is the most powerful renewable energy source for green H_2 production by PEM water electrolysis system due to the lower LCOE in the current level, leading to the lower unit H_2 production cost. Moreover, green H_2 production using solar PV and onshore wind has lower CO_2 emissions compared to grey H_2 production, but the onshore wind is more sustainable than solar PV presenting CO_2 emission improvements of 52.99% and 50.03% in current and future levels, respectively, in terms of environmental perspective (Here, the CO_2 emission for green H_2 production using solar PV-based electricity is considered as $CO_{2,ref.}$).

In particular, CO_2 emissions of solar PV, onshore wind, and hydropower for 1 kWh of electricity generation are 0.0852, 0.0245, and 0.98 kg CO_2-eq, with equal orders of CO_2 emissions for green H_2 production. Here, the hop-spots of solar PV, onshore wind, and hydropower are photovoltaic panel production consisting multi-Si water, wind turbine production being made of concrete, reinforcing steel, and low-alloyed steel, and electricity production based on hard coal, natural gas, and heavy fuel oil in power plant. Therefore, onshore wind and solar PV are more eco-friendly and sustainable than hydropower in terms of environmental aspect, although hydropower is already well known as the most powerful renewable energy source for electricity generation in terms of technical and economic aspects, owing to the largest installed hydropower energy capacity as well as the lowest LCOE in the current level.

5.4. Analytic hierarchy process

Based on unit H_2 production cost and CO_2 emissions obtained from techno-economic analysis and life cycle assessment results, respectively, for green H_2 production by PEM water electrolysis using solar PV, onshore wind, and hydropower, an analytic hierarchy process was conducted to find the most appropriate renewable energy source, in terms of techno-economic and environmental aspects, simultaneously. Fig. 37 shows the analytic hierarchy process result for green H_2 production with different weighted values of techno-economic and environmental criteria under determination at the current and future level.



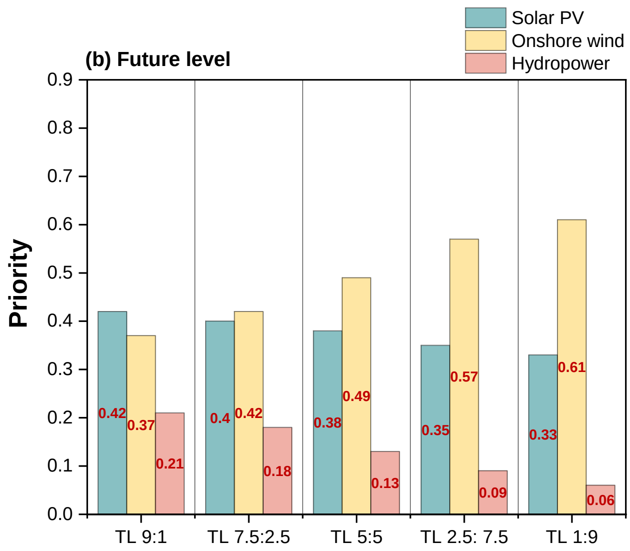


Fig. 37. Analytic hierarchy process result for green H_2 production with different weighted values of techno-economic and environmental criteria under determination in current and future level. (Here, TL 9:1 means weighted values of 9 and 1 for techno-economic and environmental criteria, respectively.)

At the current level, onshore wind is the most appropriate renewable energy source for green H_2 production whatever weighted values of techno-economic and environmental criteria are determined, in terms of economic and environmental perspectives. In addition, the next best alternative is hydropower, especially when techno-economic feasibility is the most important value to determine the alternative (i.e., TL 9:1), while hydropower becomes the worst alternative for green H_2 production if techno-economic criteria account for 50% of total weighted value. It is definitely because hydropower has the lowest LCOE leading to the lowest unit H_2 production but has a bad influence on the environment compared to others, at the current level. Therefore, in most cases (i.e., from TL 9:1 to TL 1:9), onshore wind is the best alternative and solar PV is the second-best alternative as electricity generation source for green H_2 production by PEM water electrolysis.

Next, solar PV is the best alternative, when the techno-economic result is the most important to determine the renewable energy source for green H_2 production, whereas onshore wind is the best alternative and solar PV is the second-best alternative in most cases except for TL 9:1. Furthermore, hydropower is the worst alternative as the renewable energy source for green H_2 production, in terms of techno-economic and environmental aspects, unlike the current level (Fig. 35a).

However, weighted values of techno-economic and environmental results can be decided under determination, but there are occasions when weighted values are not determined. Therefore, in this work, weighted values of both aspects were determined for multi-criteria decision analysis under uncertainty as well as under determination.

500 random numbers for the weighted value of techno-economic results ranging from 0 to 1, were generated to conduct AHP under uncertainty, and the weighted values on environmental impact were determined by calculating one minus the weighted value of techno-economic results: for example, the weighted value on environmental impact is 0.3, if the weighted value of techno-economic results is 0.7. Fig. 38 presents the distribution of count on weighted values for techno-economic and environmental results.

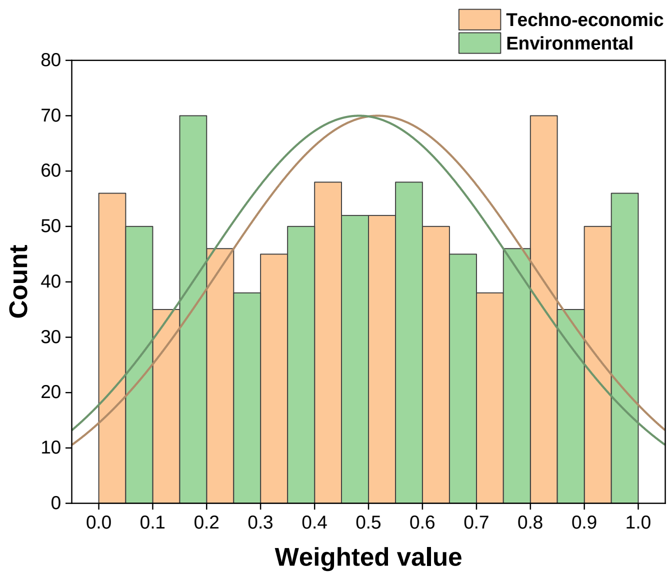


Fig. 38. Distribution of count on weighted values for techno-economic and environmental results

As shown in Fig. 38, there is the largest number of scenarios with the weighted values of 0.8 and 0.2 for techno-economic and environmental results among 500 scenarios under uncertainty (i.e., evaluation based on techno-economic results is more important than environmental impact results), although the frequency of weighted values for techno-economic and environmental results was evenly distributed. Fig. 39 presents the AHP result for green H_2 production with different weighted values of techno-economic and environmental criteria under uncertainty with distribution as shown in Fig. 38, at the current and future levels.

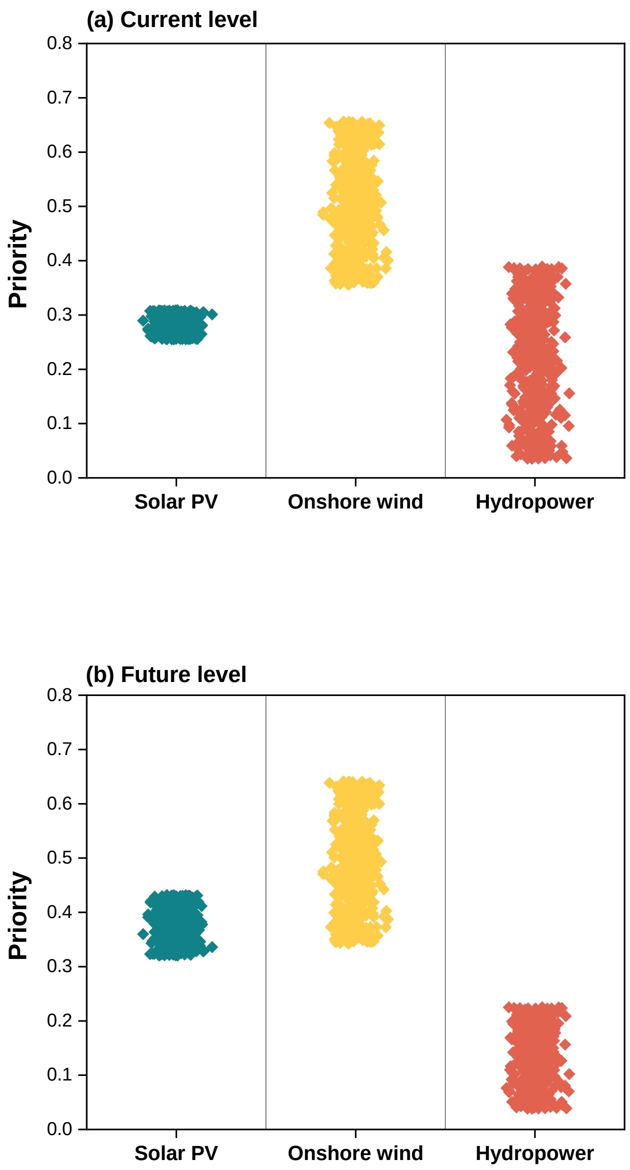


Fig. 39. Analytic hierarchy process result for green H_2 production with different weighted values of techno-economic and environmental criteria under uncertainty based on 500 random scenarios in current and future level.

First of all, Table 14 lists priority ranges of solar PV, onshore wind, and hydropower, for green H_2 production by PEM water electrolysis at current and future levels.

Table 14 Priority ranges of solar PV, onshore wind, and hydropower, for green H_2 production in current and future level

	Solar PV	Onshore wind	Hydropower
Current level	0.255–0.309	0.356–0.656	0.035-0.389
Future level	0.3221–0.432	0.343–0.641	0.038–0.225

At the current level, hydropower has wide windows on priority, due to the lowest unit H_2 production cost than others, but it has the lowest priority among three renewable energy sources for all scenarios, at the future level. It is because hydropower has higher LCOE due to the controversial environmental issues in the future. Contrarily, onshore wind has wide windows regarding priority in current as well as future levels, because of the lower unit H_2 production cost, which can make green H_2 production technology cost-competitive and economically feasible and lower environmental impacts in terms of CO_2 emission. In addition, there is a sort of overlap between onshore wind and hydropower on priority at the current level. It is when the weighted value of the techno-economic analysis result is higher than one of the environmental impact results. Moreover, the different range of priority for solar PV was identified at the current and future levels, respectively. It means the range of priority for solar PV at the future level has wider than the current one showing that solar PV becomes a more appropriate renewable energy source for green H_2 production by PEM water electrolysis.

Although solar PV has the lowest unit H_2 production cost in 2050 and H_2 economic parity can occur before 2050, from techno-economic analysis results, onshore wind is the best candidate as a renewable energy source for green H_2 production by PEM water electrolysis system when considering techno-economic and environmental aspects, simultaneously, under determination and uncertainty. Moreover, solar PV is the second-best candidate for green H_2 production in the future, owing to the high solar PV economy, when taking into account techno-economic and environmental impacts at the same time.

Reference

[1] Hydrogen production tech team roadmap (2017) https://www.energy.gov/sites/prod/files/2017/11/f46/HPTT%20Roadmap%20FY17%20Final_Nov%202017.pdf.

[2] B. Parkinson, M. Tabatabaei, D.C. Upham, B. Ballinger, C. Greig, S. Smart, E. McFarland, Hydrogen production using methane: Techno-economics of decarbonizing fuels and chemicals, International Journal of Hydrogen Energy 43 (2018) 2540-2555.

[3] K. Bareiß, C. de la Rua, M. Möckl, T. Hamacher, Life cycle assessment of hydrogen production from proton exchange membrane water electrolysis in future energy systems, *Applied Energy* 237 (2019) 862-872.

Conclusion

Recently, H_2 has been globally spotlighted to replace fossil fuels, reduce CO_2 emission, and enter the path to de-carbonization. In addition, H_2 is recognized as a promising alternative energy carrier in the future, due to its characteristics: (i) no emission of pollutants when it is burned, (ii) relatively easy and large-scale H_2 storage for a long time, and (iii) high energy efficiency. However, H_2 should be produced from chemical processes because H_2 does not exist in nature. In general, commercial H_2 production (96% of global H_2) is based on fossil fuels such as steam reforming of hydrocarbon, coal gasification, and oil/naphtha reforming, resulting in a lot of CO_2 emissions during H_2 production. In addition, many countries have been trying to install renewable energy capacity to replace fossil fuel-based energy. In this context, green H_2 production by water electrolysis using electricity generated from renewable energy sources has received much attention as an eco-friendly and sustainable alternative. However, there is a challenging problem such as high unit H_2 production cost compared to conventional one from grey H_2 production (i.e., methane steam reforming). Therefore, techno-economic analysis for green H_2 production by PEM water electrolysis using electricity generated from renewable energy sources was performed to investigate the effect of electrochemical parameters such as current density and cell active cell area on H_2 yield, determine both appropriate cases (current and future level) for economic analysis based on process simulation results, assess economic feasibility for this technology in current and future level and identify how to make unit H_2 production cost cost-competitive by considering capital and operating cost reductions such as 1) scale-up, 2) technology development of PEM water electrolysis system, 3) manufacturing cost reduction by learning-by-doing effect according to the increased global H_2 demand, and 4) the expected LCOE obtained through data fitting based on historical data.

From techno-economic analysis results, unit H_2 production costs of green H_2 production using electricity generated from solar PV, onshore wind, and hydropower were 7.345, 5.268, and 4.816 $\$\ kgH_2^{-1}$, respectively, presenting that there are higher one for all cases in current level compared to unit H_2 production cost from grey H_2 production cost of less than 2 $\$\ kgH_2^{-1}$. And, from sensitivity analysis results, electricity price is the most critical impact parameter on unit H_2 production cost and then economic insights on the increase in installed renewable energy capacity, which can lead to LCOE reduction, as well as technology development of PEM water electrolysis system are necessary to decrease unit H_2 production cost. Furthermore, there are limitations to be lower unit H_2 production cost compared to one from grey H_2 production for green H_2 production by PEM water electrolysis at the current level even if the lowest LCOE covered in this work was applied in 2050, but it can have economic feasibility for this technology in 2031 when considering the technology development as well as scale-up PEM water electrolysis system and the decreasing LCOE by 2050. Moreover, H_2 parity occurs in around 2025 (the case employing PEM water electrolysis system in current level) and 2040 (the case using PEM water electrolysis system in future level) through H_2 parity analysis. Therefore, the realization of the H_2 economy was confirmed from comprehensive economic analysis results. Although the economic aspect is an important factor to reach H_2 economy, environmental perspective should be also considered to identify this technology is eco-friendly and clean than the grey H_2 production method.

From life cycle assessment results, hydropower has higher CO_2 emissions for 1 kg H_2 production of 74.649 kgCO_2-eq. and 61.091 kgCO_2-eq. in current and future level, compared to grey H_2 production, showing that hydropower is not an appropriate renewable energy source for decarbonized H_2 production in terms of environmental aspect. Moreover, onshore wind is the better renewable energy source for green H_2 production by PEM water electrolysis system than solar PV because of the higher CO_2 emission improvement when comparing CO_2 emission for grey H_2 production, although solar PV and onshore has lower CO_2 emissions for H_2 production than grey H_2 production (8.471 kgCO_2-eq. and 7.293 kgCO_2-eq. in current and future level for solar PV and 3.982 kgCO_2-eq. and 3.644 kgCO_2-eq. in current and future level for onshore wind).

Based on techno-economic and environmental assessment results, an analytic hierarchy process was performed to determine the best alternative on renewable energy source for green H_2 production by PEM water electrolysis, when considering techno-economic and environmental perspectives, simultaneously, with different weighted values for both criteria, under determination and uncertainty. First of all, onshore wind is the most appropriate renewable energy source at the current level, for scenarios with different weighted values for each criterion under determination. And, the second-best alternative should be changed depending on the weighted values of techno-economic and environmental criteria. However, at the future level, hydropower is not an appropriate renewable energy source for green H_2 production due to the higher CO_2 emission and unit H_2 production cost caused by higher LCOE than others. Furthermore, onshore wind is the suitable candidate as a renewable energy source for electricity generation excluding the weighted value of techno-economic criterion is 9 meaning economic aspect is more critical to determine the best candidate. Next, onshore wind is the best candidate as a renewable energy source for green H_2 production by PEM water electrolysis, at current and future level, in terms of economic and environmental aspects, in the same time, when conducting AHP with weighted values for techno-economic and environmental criteria under uncertainty. However, the second-best alternative to a renewable energy source for green H_2 production should be changed depending on current and future levels as well as different weighted values of criteria.

Therefore, it can be clearly shown that the most suitable renewable energy source for electricity generation should be changed, when considering techno-economic and environmental perspectives, at the same time, although solar PV is the best alternative to renewable energy source green H_2 production by PEM water electrolysis from techno-economic analysis results and onshore wind is the most appropriate renewable energy source from life cycle assessment, in this work.